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AFWL-TR-65-143, Vol IV

AFWL-TR
65-143
Vol IV



FIREBALL PHENOMENOLOGY AND CODE DEVELOPMENT

Volume IV

SPUTTER Subroutines for Radiation Transport in Planes

General Atomic Division of General Dynamics Corporation

Special Nuclear Effects Laboratory

San Diego, California

Contract AF 29(601)-6492

TECHNICAL REPORT NO. AFWL-TR-65-143, Vol IV

July 1966

AIR FORCE WEAPONS LABORATORY
Research and Technology Division
Air Force Systems Command
Kirtland Air Force Base
New Mexico

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AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
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FOREWORD

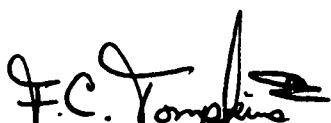
This report was prepared by General Atomic Division of General Dynamics Corporation, San Diego, California, under Contract AF 29(601)-6492. The research was performed under Program Element 7.60.06.01.D, Project 5710, Subtask 07.003/005, and was funded by the Defense Atomic Support Agency (DASA).

Inclusive dates of research were 1 June 1963 to 13 July 1965. The report was submitted 15 March 1966 by the Air Force Weapons Laboratory Project Officer, 1Lt F. C. Tompkins III (WLRT). The contractor's report number is GA-6585.

This report is divided into six volumes as follows: Volume I, Summary and the Fireball Models; Volume II, Early Fireball Phenomena in the TIGHTROPE Event;* Volume III, SPUTTER Subroutines for Radiation Transport in Spheres; Volume IV, SPUTTER Subroutines for Radiation Transport in Planes; Volume V, Material Properties; and Volume VI, Extensions of the Physics and Problem Areas.

The SPUTTER subroutines for radiation transport in planes described in Volume IV were developed by Dr. B. E. Freeman and Dr. C. G. Davis, Jr. The cooperation and contributions of Captains Milton Gillespie, William Whittaker, and George Spillman of the Air Force Weapons Laboratory are gratefully acknowledged.

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* Volume II has been withdrawn, and will not be published.

ABSTRACT

The radiation-transport subroutines of the SPUTTER code for plane slab geometry have been supplemented by alternative formulation based on integration along sampling ray paths through the slab. Angular integrations are performed by the Gaussian quadrature method which determines the ray angles. Options may be exercised to determine the number of angles and the nature of the radiation boundary condition at one boundary of the transport region. The characteristic ray code differs from the current integral method in performing problems having a large number of zones more rapidly and in having more general boundary conditions. For most applications a small number of angles give adequate accuracy. The numerical method used in the ray code is described. In addition, the organization of the code is discussed and subroutines are listed.

The SPUTTER code subroutines for radiation transport in planes described herein are as they existed on July 30, 1965. General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of these subroutines or of their description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of these subroutines for any specific use and of the validity of the information produced by their use.

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SECTION I

INTRODUCTION

The new routines for radiation transport in planes closely parallel the spherical radiation transport subroutines (Volume III) in mathematical formulation and code organization. This parallelism is especially close between the SRADTN (for spheres) and PRADTN (for planes) subroutines in which calculations peripheral to the transport integration are performed. In fact, it is likely that these subroutines can be condensed to form a single subroutine for spheres and planes, although currently they are separate.

The routines reported here are to be considered as alternatives to the routines based on the integral formulation of the transport equation currently in use. By comparison, the current integral version is more accurate in the performance of angular integrations of the intensity, but for problems requiring a large number of zones it requires more computation time. Boundary conditions on the radiation intensity, however, are much more naturally incorporated into the new version.

Conditions suggesting a preference for using the new routines are: (1) a large number of zones and a desire to reduce calculation time and (2) the necessity of specifying a radiation intensity incident on the slab surface which has arbitrary angular and frequency dependence.

The numerical sequences used in solving the transport equation are discussed in Section II. A description of the diffusion approximation used in conjunction with the transport solution is given in Section III and a brief description of the methods of frequency integration is given in Section IV. Section V includes the actual code description in terms of code organization and economics. Section VI includes some initial studies on timing and accuracy in the angular integrations.

SECTION II

NUMERICAL SOLUTION OF THE TRANSPORT EQUATION

The radiation routines described herein contain a formulation based on the numerical solution of the radiation transport equation along a selection of sampling rays through the slab. Relevant averages over the angular distribution are obtained by numerical quadrature, as described in Section 2.3, and the numerical solution of the transport equation along the photon ray is presented in Section 2.1. Criteria for selecting the sampling rays are discussed in Section 2.2. All of the derivations of this section apply to photons of a particular frequency; integration over frequency is discussed in Section IV.

The radiation transport equation in plane geometry that describes the changes in the specific intensity I_ν of photons of frequency ν resulting from pure absorption and emission according to the local thermodynamic equilibrium assumption is

$$\mu \frac{\partial I_\nu}{\partial x} = \sigma'_\nu (B_\nu - I_\nu) , \quad (2.1)$$

where

$$B_\nu = \frac{2h}{c} \frac{\nu^3}{e^{h\nu/\theta} - 1} ,$$

$$\sigma'_\nu = \sigma_\nu (1 - e^{-h\nu/\theta}) ,$$

and σ_ν is the pure absorption coefficient. The scattering coefficient is assumed to be negligibly small compared to the absorption coefficient. Additionally, the retardation of the photons is neglected, as is valid when the radiation energy is small and temperatures change slowly. The resulting equation describes the quasi-steady intensity field resulting from the distribution of sources existing at a particular time.

Defining the monochromatic optical depth, τ , as

$$\tau = \frac{1}{\mu} \int_0^x \sigma'_\nu dx , \quad (2.2)$$

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the values

$$B = a_- + b_- \tau, \quad \tau_{i-1} \leq \tau \leq \tau_{i-\frac{1}{2}},$$

where

$$a_- = \frac{B_{i-1} \tau_{i-\frac{1}{2}} - B_{i-\frac{1}{2}} \tau_{i-1}}{\tau_{i-\frac{1}{2}} - \tau_{i-1}}, \quad b_- = \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\tau_{i-\frac{1}{2}} - \tau_{i-1}} \quad (2.4)$$

and

$$B = a_+ + b_+ \tau, \quad \tau_{i-\frac{1}{2}} \leq \tau \leq \tau_i,$$

where

$$a_+ = \frac{B_{i-\frac{1}{2}} \tau_i - B_i \tau_{i-\frac{1}{2}}}{\tau_i - \tau_{i-\frac{1}{2}}}, \quad b_+ = \frac{B_i - B_{i-\frac{1}{2}}}{\tau_i - \tau_{i-\frac{1}{2}}}.$$

For the case of a constant or step-function source, the source function B takes a value dependent on which interface of the zone is affected. If the left interface ($\tau = \tau_{i-1}$) satisfies the criteria for a constant source,

$$B = B_{i-\frac{1}{2}}, \quad \tau_{i-1} \leq \tau \leq \tau_{i-\frac{1}{2}}.$$

If the right interface ($\tau = \tau_i$) satisfies the criteria,

$$B = B_{i-\frac{1}{2}}, \quad \tau_{i-\frac{1}{2}} \leq \tau \leq \tau_i.$$

The integral of Eq. (2.3) can be evaluated with the interpolation function of Eq. (2.4) to give for the intensity

$$I_i = \alpha_{i-\frac{1}{2}} + [(I_{i-1} + \gamma_{i-\frac{1}{2}}) e^{-\Delta/2} + \beta_{i-\frac{1}{2}}] e^{-\Delta/2}, \quad (2.5)$$

where

$$\alpha_{i-\frac{1}{2}} = a_+ + b_+ (\tau_i - 1),$$

$$\beta_{i-\frac{1}{2}} = a_- - a_+ + (b_- - b_+) \left(\tau_i - \frac{\Delta}{2} - 1 \right),$$

$$\gamma_{i-\frac{1}{2}} = b_- (1 + \Delta - \tau_i) - a_-.$$

In these expressions, $\Delta = \tau_i - \tau_{i-1}$. The coefficients of Eq. (2.5) can be re-expressed by using the definitions of Eq. (2.4):

$$\left. \begin{aligned}
 \alpha_{i-\frac{1}{2}} &= B_i - \frac{B_i - B_{i-\frac{1}{2}}}{\Delta/2}, \\
 \beta_{i-\frac{1}{2}} &= \frac{B_i - B_{i-\frac{1}{2}}}{\Delta/2} - \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\Delta/2}, \\
 \gamma_{i-\frac{1}{2}} &= - \left(B_{i-1} - \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\Delta/2} \right).
 \end{aligned} \right\} \quad (2.6)$$

The terms in Eq. (2.6) may be interpreted as containing combinations of numerical approximations to the values of the source function and the τ derivative of the source function at the boundaries of the interval.

This form of the equation, in fact, can be obtained in another way starting from Eq. (2.3). Two successive integrations by parts transforms the expression for I_i into the following equivalent form:

$$I_i = \left(B - \frac{\partial B}{\partial \tau} \right)_i + \left[I_{i-1} - \left(B - \frac{\partial B}{\partial \tau} \right)_{i-1} \right] e^{-\Delta} + \int_{\tau_{i-1}}^{\tau_i} \frac{\partial^2 B}{\partial \tau^2} e^{-(\tau_1 - \tau)} d\tau, \quad (2.7)$$

in terms of values of the source function and the first two derivatives of the source function with respect to τ .

In an optically thin interval, the most important contribution arises from the terms I_{i-1} and B , which represent the transmitted intensity and the emission from the zone. The derivative terms cancel in this approximation; this is perhaps more directly indicated by Eq. (2.3). In the optically thick interval, which is the extreme opposite, only the first two terms evaluated at i are usually of significance. The terms from $i-1$ are strongly attenuated and $\partial^2 B / \partial \tau^2$ in the integral is usually small. In the limit, the diffusion approximation results from the term $\partial B / \partial \tau)_i$. Between limits, it is necessary to consider the integral term in Eq. (2.7).

If Δ is not too large, a representative mean value of the exponential in the interval may be taken to give for the integral of Eq. (2.7)

$$\int_{\tau_{i-1}}^{\tau_i} \frac{\partial^2 B}{\partial \tau^2} e^{-(\tau_1 - \tau)} d\tau \approx e^{-\Delta/2} \left[\left(\frac{\partial B}{\partial \tau} \right)_i - \left(\frac{\partial B}{\partial \tau} \right)_{i-1} \right],$$

and thus the expression for intensity becomes

$$I_i = \left(B - \frac{\partial B}{\partial \tau} \right)_i + \left\{ \left[I_{i-1} - \left(B - \frac{\partial B}{\partial \tau} \right)_{i-1} \right] e^{-\Delta/2} + \left[\frac{\partial B}{\partial \tau} \right]_i - \left[\frac{\partial B}{\partial \tau} \right]_{i-1} \right\} e^{-\Delta/2} . \quad (2.8)$$

This expression has just the form of Eqs. (2.5) and (2.6) when the difference expressions are identified with the derivatives.

It is clear from the derivation of Eq. (2.5) that the resulting intensity is a positive quantity. With positive values for zone source functions, the linear interpolation expression assures that the integral contribution is always positive. Since the boundary intensity is always a positive quantity, the positivity of all intensities is assured.

In the diffusion approximation limit, only quantities at interface i will survive, and

$$I_i = B_i - \frac{\partial B}{\partial \tau} \Big|_i ,$$

which can be evaluated as

$$\frac{\partial B}{\partial \tau} = \mu \frac{\partial B}{\partial h} , \quad (2.9)$$

where

$$h = \int_0^x \sigma' dx .$$

The independent variable h depends only on x , so that angular integrations of I_i can be performed explicitly in the diffusion approximation, which takes account of the dependence on angle of Eq. (2.9). A difference approximation can also be based on this expression, assuming that B is linear in h , i. e.,

$$\frac{\partial B}{\partial \tau} \Big|_i \cong \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}} \mu . \quad (2.10)$$

where μ is the cosine of the angle which the ray makes with the slab normal. The corresponding equation for the intensity is Eq. (2.5), in which

$$\begin{aligned}
 \alpha_{i-\frac{1}{2}} &= B_i - \nu \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}}, \\
 \beta_{i-\frac{1}{2}} &= \mu \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}} - \mu \frac{B_{i-\frac{1}{2}} - B_{i-1}}{h_{i-\frac{1}{2}} - h_{i-1}}, \\
 \gamma_{i-\frac{1}{2}} &= - \left(B_{i-1} - \mu \frac{B_{i-\frac{1}{2}} - B_{i-1}}{h_{i-\frac{1}{2}} - h_{i-1}} \right),
 \end{aligned} \tag{2.11}$$

2.1.2. Small-optical-depth Expansion

If the optical depth is very small, the intensity expression in Eq. (2.3) takes a much simpler form,

$$I_i = I_{i-1} + \left[\frac{1}{4} B_i + \frac{1}{4} B_{i-1} + \frac{1}{2} B_{i-\frac{1}{2}} - I_{i-1} \right] \Delta. \tag{2.12}$$

Although this result is the limiting form of Eqs. (2.5) and (2.6), the terms must cancel through second order in an expansion in Δ before the first surviving term, derived in part from the quadratic terms of the exponentials, is obtained. Consequently, for sufficiently small argument, the finite number of figures used in the exponential will render the result inaccurate. For the exponential from the IBM-7044 system, this restricts the argument to a number greater than $\sim 2 \times 10^{-4}$; but with the lower-accuracy fast exponential (see Section V), the argument must be somewhat larger. Since the relative error approximately equals the argument of the exponential, the criterion for using Eq. (2.12) in the PTRANS subroutine is now set at $\Delta \leq 2 \times 10^{-2}$. With this value, the greatest relative error arising from the expansion and cancellation should be on the order of 1 percent.

2.1.3. Boundary Conditions

Integration of the transport equation to obtain intensities is performed through the thickness of a zone, called a "trans" region. At intersections of characteristic rays with the inner and outer surfaces of each layer it is necessary to supply the starting value of the intensity I_{i-1} required in Eq. (2.5). Three classes of boundary conditions occur:

1. The trans region outside boundary coincides with outside zones of the SPUTTER calculation and a prescribed function, I_0 , is applied at the left boundary value:

$$I(X_{IA+1}, \mu) = I_0, \quad \mu \leq 0 \text{ or blackbody boundary condition.} \tag{2.13}$$

2. The right-hand boundary of the slab provides for reflective and transmittal boundary conditions as well as special routines to establish prescribed intensities for angles with $\mu < 0$ at the boundary:

$$I(X_{IB}, -\mu) = I(X_{IB}, \mu), I(B_{IB}, \mu) = 0, \quad (2.14)$$

or

$$I(B_{IB}, -\mu) = I_0(\mu, t),$$

where I_0 is the prescribed negatively directed boundary intensity applied to the outer boundary as a function of angle, frequency, and time. Intensities at up to 50 frequencies and six angles can be accommodated in the table located in the array QINT1(N). The table entries are used as I_0 and are formed in the subroutine QUE4 where they are stored in the QINT1 array. Since this subroutine is appropriate to the thermal interaction application, additional uses may require subroutines tailored to the specific application.

3. All other trans boundaries are bounded by regions in which the diffusion approximation is valid (see Section III). Consequently, the boundary surface intensities on contiguous trans regions inside or outside of a diffusion region are given by the diffusion approximation intensity derived in Section III:

$$I_{i-1} = B_{i-1} - \mu \frac{\partial B}{\partial h}_{i-1} \quad (2.15)$$

2.2. ANGULAR INTEGRATION

Integrals over the polar angle of the intensity are required, as described in Section 2.2.1, to carry the calculation forward in time and to provide edits of informative derived quantities. These are formed by numerical quadrature using the intensities evaluated at a series of discrete values of polar angle by the integrations described in Section 2.2. Since in the plane calculation the value of the polar angle remains fixed along a characteristic ray and enters only parametrically in the equations, it is possible to exercise a choice of polar-angle values in order to optimize the accuracy of the resulting integrals.

The numerical quadrature method used for the PTRANS subroutine is the so-called double Gaussian.⁽¹⁾ In this method the integrals of the radiation quantities (flux, energy, pressure, etc.) are approximated by

$$\int I f(\mu) d\mu = \sum_0^n A_m (I f)_m,$$

where $(If)_m$ is the known value of the integrand at a chosen value μ_m of the cosine of the polar angle, μ . In the method of Gaussian, not only are the coefficients A_m determined but the values of μ_m are fixed to minimize the difference between the integral and the approximation. The result of this minimization is to relate the μ_m to the zeros of the Legendre polynomial of order $n + 1$.

For those integrals having the range $-1 \leq \mu \leq 1$ it is frequently advantageous to treat the forward and backward hemispheres separately to allow for the possibility of a discontinuity in I at $\mu = 0$. Such discontinuities or very abrupt changes in the values of the intensity between forward and backward directions may occur in systems which are transparent enough that strong source regions are accessible. In these cases, a better fit to the integrand is obtained by the two approximating functions which permit a discontinuity at $\mu = 0$ than by a single approximating function which imposes a smooth behavior near $\mu = 0$. The method used in PTRANS, based on separate integration regions for $-1 \leq \mu \leq 0$ and $0 \leq \mu \leq 1$, is called the double Gaussian quadrature method. Values of A_m and μ_m are derived by a simple transformation from those for the single integration region. Since the angles for a single integration region are arranged symmetrically about the interval midpoint, for double region integration it is possible to identify pairs of angles $\pm \mu_m$ having the same weight A_m . In Table 2.1, the values⁽²⁾ for the $0 \leq \mu \leq 1$ interval are recorded for values of $n = 1, 2, 3, 4, 5$. The total number of forward and backward angles, $2n + 2$, for each n (also equal to the total number of entries in the table of μ_m and A_m for each n) is also listed in the table.

The backward and the corresponding forward ray integrations in the PTRANS subroutine are performed sequentially. Since the same absolute values of μ_m are required for these two calculations, many of the quantities formed in the backward integration pass can be used for the forward pass as well, and hence these quantities are saved to increase calculation efficiency. Contributions of the pair of forward and backward intensities to the weighted sums corresponding to the angular integrals are tallied at the same time that the forward integration pass is being calculated.

Table 2.1
GAUSSIAN WEIGHTS

$n = \text{LMDA}(37)-1$	Total No. of Angles, $2n+2$	$\mu_m = \text{RR(NMU)}$	A_m	$\mu_m A_m = \text{RR(NGS)}$
1	4	0.2113248	0.5	0.1056624
		0.7886752	0.5	0.3943376
	6	0.1127017	0.2777778	0.03130603
		0.5	0.4444444	0.2222222
	8	0.8872983	0.2777778	0.2464718
		0.0694318	0.1739274	0.0120761
3	8	0.3300095	0.3260726	0.1076071
		0.6699905	0.3260726	0.2184655
	10	0.9305682	0.1739274	0.1618513
		0.0469101	0.1184634	0.00555713
4	10	0.2307653	0.2393143	0.055225436
		0.5	0.2844444	0.1422222
		0.7692347	0.2393143	0.1840889
	12	0.9530899	0.1184634	0.1129063
		0.0337652	0.0856622	0.00289240
		0.1693953	0.1803808	0.03055566
5	12	0.3806904	0.2339570	0.0890652
		0.6193096	0.2339570	0.1448918
		0.8306047	0.1803808	0.1498251
		0.9662348	0.0856622	0.0827698

SECTION III

THE DIFFUSION APPROXIMATION

The radiation transport equation in the limiting case of an optically thick medium admits of the diffusion approximation in which the expression for the radiation intensity is greatly simplified; only the local properties affect the radiation intensity at the point in question. An expansion of the radiation source function B_ν about the point r permits the intensity $I_\nu(\mu)$ of the radiation field in the direction making an angle, whose cosine is μ , with the linear direction to be formed.

3.1. DIFFERENTIAL FORM OF THE DIFFUSION FLUX

The general solution of the transport equation forms the starting point of the derivation. The integral expression for the intensity applicable to all geometries is

$$I(\tau) = \int_{-\infty}^{\tau} B(\tau') e^{-(\tau-\tau')} d\tau' ,$$

where $\tau = \int_0^x \kappa_\nu \rho ds$, in which κ_ν is the monochromatic absorption coefficient (in cm^2/g) at frequency ν . By expanding $B(\tau')$ in series about the point τ , i. e.,

$$B(\tau') = B(\tau) + \frac{\partial B}{\partial \tau} (\tau' - \tau) + \frac{1}{2} \frac{\partial^2 B}{\partial \tau^2} (\tau' - \tau)^2 + \dots ,$$

the intensity becomes

$$I = B - \frac{\partial B}{\partial \tau} + \frac{1}{2} \frac{\partial^2 B}{\partial \tau^2} - \dots$$

or

$$I = B - \frac{\mu}{\kappa_p} \frac{\partial B}{\partial x} + \frac{\mu^2}{\kappa_p} \frac{\partial}{\partial x} \left(\frac{1}{\kappa_p} \frac{\partial B}{\partial x} \right) - \dots$$

for plane slab geometry.

The diffusion approximation results from retention of only the first two terms, so that the diffusion intensity is

$$I = B - \frac{\mu}{\kappa_p} \frac{\partial B}{\partial x} \quad (3.1)$$

and the monochromatic diffusion flux ϕ_r and radiation energy E_R are

$$\phi_r = 2\pi c \int_{-1}^1 I \mu \, d\mu = - \frac{4\pi c}{3} \frac{1}{\kappa_p} \frac{\partial B}{\partial x}, \quad (3.2)$$

$$E_R = 2\pi \int_{-1}^1 I \, d\mu = 4\pi B.$$

3.2. CRITERIA FOR THE SELECTION OF DIFFUSION REGIONS

The criteria for the validity of the diffusion approximation can be obtained by examination of the above derivation--namely, that the expansion of the source function be justified and that the expansion converge rapidly so that the neglect of all but the leading terms is valid. If the source function is linear in τ' at the point in question and is also linear for a distance of the order of one mean free path on either side of the point, the criteria are satisfied. These criteria are difficult to quantify since they refer to a finite region containing the point in question. If all of the terms (or a large number of them) were checked for rapid convergence, this would imply (making a smoothness assumption) that the diffusion criterion is met. It is not possible with finite differences, however, to form the higher-order local derivatives approximations.

In the SPUTTER subroutine PRADTN, criteria designed to give an indication of both the local and nonlocal behavior have been employed. First, at the zone interface at which the intensity and flux are to be evaluated, the inequality

$$\left| \frac{\partial B}{\partial h} \right| \ll B \quad (3.3)$$

is required. In this expression $h = \int \kappa_p \, dx$ is the optical depth normal to the slab; the derivative is approximated by the centered first difference of B between adjacent zones. The resulting expression, of course, contains some nonlocal aspects resulting from the finite difference approximation, which ensures that when neighboring zones are optically thick, no nonlocal source perturbation is close enough to invalidate the diffusion approximation. However, to provide for the cases when a source perturbation is located a fraction of an optical depth from an interface meeting the condition of Eq. (3.3), the diffusion region is constricted. Starting from the closest

interfaces outside the diffusion region (where Eq. (3.3) is not satisfied), all of those interfaces lying within a prescribed number of mean free paths are removed from the diffusion region.

The criteria used in SPUTTER are controlled by input numbers. The criterion of Eq. (3.3) uses the input number HCB:

$$|TG| < HCB \times Y2 , \quad (3.4)$$

where TG is the difference approximation to the gradient and Y2 is the source function evaluated at the interface by interpolation. The second criterion uses the input number HVB (in mean free paths). If

$$|Q3(I) - Q3(J)| > HVB , \quad (3.5)$$

then the interface with index J which satisfies Eq. (3.4) is removed from the diffusion region. In Eq. (3.5), Q3 is the normal optical depth and I is the index of the nondiffusion interface adjoining the diffusion region.

Although the diffusion calculation is considerably faster than the transport, the establishment of two transport regions separated by the single zone requires still more calculation to set up characteristic rays and perform bookkeeping operations. To avoid the duplicate setup calculations required for an additional transport region, a test is made to eliminate a diffusion region consisting of a single zone.

3.3. DIFFERENCE FORM OF THE DIFFUSION FLUX

The diffusion intensity derived above is

$$I = B - \frac{\mu}{\kappa \rho} \frac{\partial B}{\partial x} .$$

In the group frequency approximation of SPUTTER, the intensity integrated over a frequency interval (ν_j, ν_{j+1}) is required:

$$\int_{\nu_j}^{\nu_{j+1}} I d\nu = \int_{\nu_j}^{\nu_{j+1}} B d\nu - \frac{\mu}{\rho} \frac{\partial B}{\partial x}^4 \int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta}^4 \frac{d\nu}{\kappa} .$$

In terms of the partial Rosseland mean absorption coefficient

$$\kappa_j = \frac{\int_{v_j}^{v_{j+1}} \frac{\partial B}{\partial \theta^4} dv}{\int_{v_j}^{v_{j+1}} \frac{\partial B}{\partial \theta^4} \kappa_v}.$$

the frequency group intensity becomes

$$I_j = \int_{v_j}^{v_{j+1}} I dv = \int_{v_j}^{v_{j+1}} B dv - \frac{\mu}{p} \frac{\partial \theta^4}{\partial x} \frac{\int_{v_j}^{v_{j+1}} \frac{\partial B}{\partial \theta^4} dv}{\kappa_j}. \quad (3.6)$$

It is desired to evaluate this quantity at each zonal interface in the mesh. Since the known quantities are the zone temperatures and densities, the absorption coefficients κ_j and the integrated source functions $X_6 = \int B dv$ are first evaluated, not at the interfaces but at positions representative of each zone.

The question remains as to how best to approximate the derivatives and interpolate for the coefficients in Eq. (3.6) at the interfaces from the quantities available at zone positions. The answer depends on the temperature and density profile across the interface from which these terms could be calculated directly. Since the profile is not known, we must select a reasonable approximation which will permit the calculation to be carried out. In fact, the appropriate profile depends on the events which have taken place in the calculation and on the energy transport mechanisms of greatest importance in it. As extreme examples, a problem dominated by hydrodynamics might have quantities determined by passage of a strong shock and subsequent linearization in mass coordinates of the pressure behind the shock, whereas a radiation-dominated diffusion problem is characterized by linearity of the radiation potential, which, in turn, depends on the Rosseland opacity. Of course, such detailed information about the progress of a problem is generally unavailable, so, at best, an approximation based on over-all accuracy is needed.

Since the terms under consideration are the radiation diffusion equations, the interpolation is performed in a way to give greatest accuracy when the diffusion terms are most important--namely, when the profile is being determined entirely by radiation diffusion. It is also desirable to reduce the number of coefficients requiring interpolation. This can be done by noting the identity

$$\frac{\partial}{\partial x} \int_{v_j}^{v_{j+1}} B dv = \frac{\partial \theta^4}{\partial x} \int_{v_j}^{v_{j+1}} \frac{\partial B}{\partial \theta^4} dv$$

and by forming the variable $\tau = \int \rho \kappa_j dx$. In terms of these quantities, the intensity can be written as

$$I_j = \int_{v_j}^{v_{j+1}} B dv - \mu \frac{\partial \int_{v_j}^{v_{j+1}} B dv}{\partial \tau}$$

SECTION IV

FREQUENCY INTEGRATION

Equations derived in Sections II and III which are applicable to a particular frequency of the radiation field are of limited usefulness in the SPUTTER calculations. Although in principle a calculation at a particular frequency might be valuable for comparison with high-resolution spectroscopy, in practice no such data have been available. Of much more use are intensities averaged over a wide frequency band. These quantities can be compared with data from wide-band measurements and, most important of all, can be summed for use in the energy integration in the SPUTTER code. The quantities to be summed are the frequency-integrated radial flux component, the radiation energy density, and the radiation pressure. For performing interaction calculations, it is also valuable to form other components of the radiation flux.

Basically, the quantity which is required for each of the above applications is the frequency-group intensity I_{ij} ,

$$I_{ij} = \int_{\nu_j}^{\nu_{j+1}} I_i d\nu . \quad (4.1)$$

Then, for example, this quantity can be integrated over angles to form ϕ_{ij} , the contribution to the flux at position i of frequency group j:

$$\phi_{ij} = \int_{-1}^1 (I_{ij}^+ - I_{ij}^-) \mu d\mu ,$$

and thus the total radiant flux at position i is

$$\phi_i = \sum_j \phi_{ij} .$$

Equation (2.8) gives the expression for the frequency-dependent intensity to be used in Eq. (4.1). The frequency integration of Eq. (2.8) has been reported recently,⁽⁴⁾ but the current SPUTTER code does not include the transmission functions. The first two terms of Eq. (2.8) which form the diffusion limit can be integrated, as in Section 3.3, to give

$$I_{ij} = B_{ij} - \frac{\mu}{\sigma R_j} \frac{\partial B_{ij}}{\partial x} \quad (\text{diffusion limit}), \quad (4.2)$$

in which the first term

$$B_{ij} = \int_{v_j}^{v_{j+1}} B_i(v) dv$$

is the frequency-group Planck function and the second term contains the frequency-group Rosseland mean absorption coefficient $\sigma R_j = \rho \kappa_j$. In this form, Eq. (4.2) correctly gives the frequency-group intensity for the optically thick limiting case. The remaining B_i and $\partial B / \partial x$ terms of Eq. (2.8) are formed in the same way. Thus,

$$I_{ij} = B_{ij} - \left(\frac{\mu}{\sigma R} \frac{\partial B}{\partial x} \right)_{ij} + \left[\left(\frac{\mu}{\sigma R} \frac{\partial B}{\partial x} \right)_{ij} - \left(\frac{\mu}{\sigma R} \frac{\partial B}{\partial x} \right)_{i-1,j} \right] \overline{e^{-\Delta/2}} + \left[I_{i-1,j} - B_{i-1,j} + \left(\frac{\mu}{\sigma R} \frac{\partial B}{\partial x} \right)_{i-1,j} \right] \overline{e^{-\Delta}}. \quad (4.3)$$

In Eq. (4.3), mean values of the exponentials have been extracted from the frequency integrals and the outstanding problem is to specify their values. Two options are available; they differ in the absorption coefficient used to calculate the optical depth. The first is

$$\overline{e^{-\Delta}} = e^{-\sigma R \delta} \quad (4.4)$$

and the second is

$$\overline{e^{-\Delta}} = e^{-\sigma P \delta},$$

where

$$\sigma P = \frac{\int_{v_j}^{v_{j+1}} \sigma_v B_v dv}{B_{ij}}$$

and

$$\delta = x_i - x_{i-1}.$$

For small optical depth, the correct result makes use of the Planck mean absorption coefficient. From Eq. (2.12) the frequency integration then gives

$$I_{ij} = I_{i-1,j} + \left[\frac{1}{4} B_{ij} + \frac{1}{4} B_{i-1,j} + \frac{1}{2} B_{i-\frac{1}{2},j} - I_{i-1,j} \right] \sigma_p \delta . \quad (4.5)$$

The above prescriptions for frequency-group means are far from satisfying and call for further work. Considerable economies can be made through reductions in the number of frequency groups if a more accurate means of averaging within groups can be found. Presently used choices of frequency groups appear to give a reasonably accurate result, however, as indicated by comparisons between calculations with the nominal number of frequency groups and calculations with a very large number of frequency groups. (It is expected that a unique correct result will be obtained as the number of frequency groups is increased, irrespective of the choice of the weighting function in the frequency-group-average absorption coefficient.) Consequently, a very few frequency groups should be adequate if a suitable averaging procedure were developed.

Even with a crude averaging scheme, considerable improvement in accuracy results from choice of frequency-group boundaries so as to reduce the variation of the absorption coefficient within the group.

Work on the absorption coefficient for air indicates that approximately 20 groups, carefully selected as to their locations, afford quite adequate resolution. Enough information is known about air to make this selection appear quite reasonable. Air absorption coefficient tapes (DIANE)* have been prepared for 18, 20, and 90 groups. The 90-group tape is used to check on the frequency integrations at selected times. The proper averages to use are difficult to decide on at this time. There are provisions for reading into storage from the DIANE tapes both the Rosseland and Planck averages, which are used at present in the thick or thin limits, respectively.

* See Section VI of Volume V.

SECTION V

SUBROUTINE ORGANIZATION AND ECONOMICS

The present plane transport subroutines were written with the idea of removing unnecessary calculations from inside the frequency loop and characteristic ray integrations. These improvements required an increase in storage for the subroutines to attain a decrease in calculational time. The reorganized subroutines will be discussed in two sections, corresponding to the two major subroutines: (1) the radiation subroutine (PRADTN) in which most of the preliminary setup and the diffusion calculation is completed and (2) the transport subroutine (PTRANS) in which the intensity calculation and angular integrations are performed. The subroutines which execute the opacity interpolations (KAPPA), Planck function (PLNKUT), and fast exponential (FREXP) will be discussed in Section 5.4. The input numbers and the output edits will be presented in Sections 5.5 and 5.6.

5.1. THE PRADTN SUBROUTINE

In PRADTN, the high-frequency groups are merged, a source region is established, boundary sources and derivatives are calculated, regions for transport and diffusion are formed, diffusion fluxes are calculated, frequency integration is performed, and the radiation time-step control is evaluated. Each of these activities in PRADTN will be discussed in subsequent paragraphs.

5.1.1. Merge Frequency Groups

Frequency groups that are too far out on the Planck tail for a "maximum" temperature in the mesh are merged. The criterion used is as follows: If the lower frequency boundary $h\nu_1$ of the group in question ($h\nu_1$, $h\nu_2$) is greater than ten times the maximum temperature (THMAX) in the mesh, this group will be merged with the next lower group. Merging will continue until over half the groups have been merged; at this point, either the calculation is terminated or a second DIANE tape is called. On merging, Rosseland and Planck averages are formed by using the following equation for $dB/d\theta^4$ and the appropriate sums:

$$\frac{dB_{\nu}}{d\theta^4} \cong \frac{0.0384974}{\theta^4} \left[\left(\frac{h\nu_2^4}{1 - e^{-h\nu_2/\theta}} \right) e^{-h\nu_2/\theta} - \left(\frac{h\nu_1^4}{1 - e^{-h\nu_1/\theta}} \right) e^{-h\nu_1/\theta} \right],$$

$$\sum b_j \theta^4, \sum \frac{dB_{\nu}}{d\theta^4}, \sum b_j \theta^4 \kappa_P, \text{ and } \sum \frac{dB_{\nu}}{d\theta^4 \kappa_R}. \quad (5.1)$$

The Planck weighting functions (b_j) are obtained from PLNKUT, as described later. On completing the merging, the merged opacities are formed:

$$\overline{\kappa_R} = \sum \frac{dB_{\nu}/d\theta^4}{\sum dB_{\nu}/(d\theta^4 \times \kappa_R)} \quad (\text{CAPAR}), \quad (5.2)$$

$$\overline{\kappa_P} = \sum \frac{b_j \theta^4 \kappa_P}{\sum b_j \theta^4} \quad (\text{CAPAC}).$$

5.1.2. Set Up Sources and Derivatives

The frequency-dependent sources must be established at the interfaces from the zonal quantities $b_j \theta_{i+\frac{1}{2}}^4$ ($X6(i)$) and $\tau_{i+\frac{1}{2}}$ ($H3(i)$). The difference equations used were given in Section 2.1. Before the calculation of the Planck function (b_j) is made, i. e., before calling PLNKUT, a test is made to see if u_1 (i. e., the reduced frequency $h\nu_1/\theta \geq 19$; if so, $b_j = 0$ (i. e., the source $X6(i) = 0.0$). If $u_1 < 19.0$ and $u_2 \leq 0.01$, then $b_j = 0$ also, assuming that for $\theta^4 < 10^5$, the small b_j ($b_j \sim 10^{-5}$) will produce a negligibly small source contribution. An index (ICX) is set equal to the last zone that contains a source. This source index is used to limit the transport calculation to the region containing sources. While setting up the sources and derivatives, tests are made on their discontinuous nature to use either a linear or constant form in the intensity integrations. The initial check is on the minimum optical depth of adjacent zones to ensure that both are transparent (less than 0.3). If this condition holds and if both the sources and optical depths are changing rapidly in x (change greater than a factor of two), the derivative at that interface ($TC(i)$) is set equal to zero. The zero source derivative is used in PTRANS, as a test, to set up the constant source terms. For the intensity integration, special boundary sources and derivatives are also established at the edge of the source region ($I = ICX$) and at the outside of the mesh ($I = IM$) (see Section 2.1.3).

5.1.3. Determine Diffusion Region

The principal criterion for defining a diffusion region is that the first derivative of the source function (TG) be small compared to the source (Y2) (see Section 3.2). When the zone is found to be diffusion, the boundary is tagged by setting (X3 = -1.). Before incorporating this interface into a diffusion region, the possible influence from sources on either side is considered and a further test is made. From the last diffusion boundary, a test is made for an optical depth in succeeding zones to the left. If more than HVB optical depths appear in the next zone, then this zone is calculated by transport and removed from the diffusion region (set X4(i) = -1.0). HVB is an input number, which is usually around 5. When $x = 0$ is reached after testing each zone, zones out to the right of the present transport region are tested in the same manner. The above test buffers the transport region with an (HVB) mean-free-path-thick diffusion boundary. If the zone boundary stays diffusion, i.e., $X3(i) = -1.0$ and $X4(i) = 0.0$, a diffusion flux is calculated from the source gradients, as described in Section 3.1. The regions where $X3(i) = 0.$ or $X3(i) = -1.$ and $X4(i) = -1.$ have been established as transport regions because they did not meet the diffusion criteria or they reverted to transport regions by the optical-depth test described above. This transport region is then identified by setting the left boundary to IAX and the right boundary to IBX. More than one trans region may be set up in PRADTN, and if so, a PTRANS calculation will be made for each region. No one-zone diffusion region is allowed and the region outside the sources ($I > ICX$) is always considered a transport region.

5.1.4. Time-step Control and Monofrequency Calculation

These two aspects of the new code are related since the "grey" absorption coefficients from the DIANE tape are used to estimate a radiation time step as well as to form the monofrequency time-dependent calculation. In the multifrequency calculation, after all groups have been processed, an additional call for KAPPA is made to read in the grey absorption coefficients. These averages were obtained by integrating the frequency-dependent absorption coefficients for both Planck (κ_p) and Rosseland (κ_R) in the DIANE code. The actual time step for radiation transfer is then obtained from the formula

$$\Delta t_R = (0.5 + 1.5 H3(i)^2) / (ac \kappa_R \theta^3) \times CV(i) , \quad (5.3)$$

where $CV(i)$ is the specific heat and $ac = 4.12 \times 10^{12}$. The mass point in question is also checked to ensure that it will not gain or lose more than half its original energy:

$$\Delta t_R = 0.5 \times CV(i) \times \theta(i) \times G(i) / |ER(i)| , \quad (5.4)$$

where $\mathbf{E}\mathbf{R}(i)$ is the divergence of the flux and $\mathbf{G}(i)$ is the mass in the zone. The minimum of these values is compared to the hydro time step (Courant) and if smaller,

$$\mathbf{NRAD} = \text{FIX}(\mathbf{DTH2}/\mathbf{DTRMIN}) \quad \text{and} \quad \mathbf{DTR} = \mathbf{DTH2}/\mathbf{NRAD} \quad (5.5)$$

is set to cycle NRAD times through the radiation routine.

The monofrequency calculation also uses the grey absorption coefficients from the DIANE tape. If $KMAX = 0.0$ and $S15 = 1.0$, the frequency-averaged opacities are bypassed on the tape and only the grey absorption coefficients are read into storage. For succeeding cycles, $S15$ is set equal to zero and the interpolations for κ_R and κ_P are performed in KAPPA using the stored opacities originally read into KAPPA's common storage. When the problem is restarted it is therefore necessary to reload $S15$ equal to one. If the DIANE tape is not designated (the tape unit assigned must be stored in $AMASNO(J+17)$, where J is the material number), then the KAP routine is called (KAP8 for air) and used for the monofrequency calculation.

5.2. THE PTRANS SUBROUTINE

The subroutine PTRANS is called by PRADTN to carry out the intensity integration between IAX and IBX , saving various quantities on the inward pass that will be used on the outward pass as well as the angular integration of the flux between rays ($\int_{-1}^1 I\mu d\mu$). After the intensity transport along a typical ray in the outward direction ($iA \rightarrow iB$) is done, the flux is calculated while the inward pass of the intensity calculation is being completed. The angular integration is based on a linear interpolation of the intensities between rays. The logic in PTRANS is described in detail in the following sections.

5.2.1. Selection of Angles

At present, only five sets of Gaussian angles and weights are stored in the subroutine. These can be selected by setting an input number ($LMDA(37)$, the number of angles with $\mu > 0$) to the desired $n+1$. The selection from storage is made from the following indices

$$NY = LMDA(37) - 1$$

$$NMU = (NY-1) \times (NY+2) + 1$$

$$NGS = NMU+NY + 1 ,$$

NMU selects the cosine of the angle (μ_m); NGS selects the relation ($\mu_m A_m$), the cosine of the angle times the Gaussian weights for the flux formulation.

5.2.2. Intensity Integration along Characteristic Rays

The integration using Eq. (2.11) starts at the left boundary with the appropriate boundary condition and proceeds outward, storing the exponentials $e^{-\Delta\tau}$ in (H4(i)), the derivatives $\mu \partial B / \partial h$ in X8(i), and the calculated intensities in sum X3(i). The more general boundary conditions are established (see Section 2.1) and the stored quantities are now used except for the change of sign of $\mu \partial B / \partial h$ in Eq. (2.1) to calculate the intensities I(F2), on the outward pass.

The regions where constant sources, and therefore zero boundary derivatives, should be used in the intensity integrations were established in PRADTN by setting TG(i) equal to zero. In the integration along a particular ray, a test is made on TG(i) at each interface; if zero, the source terms Y2(i - 1) and Y2(i) are set equal to $X6(i - \frac{1}{2})$ respectively (see Fig. 2.1).

As discussed in Section 2.1.1, the accuracy of the exponential term and the effect of truncating errors mean that the general formula will not reduce in the limit of small optical depths to the transparent case. To correct this situation, a test is made on τ_i (the half optical depth τ is stored in H2(i)), and if $\tau < 10^{-2}$ a switch is made to the limiting form of the transport equation (Eq. (2.12) developed in Section II).

5.2.3. Angular Integration

The only integral over angle formed in PTRANS, at present, is the flux; ($\int I \mu d\mu$) the formula for energy ($\int I d\mu$) is included for possible use later. These integrals are formed on the outward pass from the intensity (sum X3(i)) stored on the inward pass and the intensity being calculated (F2). The difference forms of the equations are

$$X2(i) = \sum (F2 - \text{sum } X3(i)) \times \mu_m A_m ,$$

$$ER(i) = \sum (F2 + \text{sum } X3(i)) \times A_m .$$

5.3. DIFFERENCES WITH INTEGRAL FORMULATION

The principal difference in the subroutines is in replacing the integration of angle done explicitly in the integral formulation by a sampling scheme of a double Gaussian nature. It is expected that accuracy can be achieved with a minimum number of rays (presumably less than $n = 6$, see Section 2.2). This result is in logical agreement with the use of the S4 approximation in the neutron-transport work. The advantage, therefore, will appear in problems with many zones, since the integral method will

increase as the number of zones squared whereas the present method will only increase linearly with zones. Furthermore, the present method makes it possible to have special boundary conditions depending on angle (see Section 2.1.3).

5.4. AUXILIARY SUBROUTINES

In addition to the two new basic subroutines PRADTN and PTRANS, some changes have been made in the auxiliary subroutines EXP, PLNKUT, and KAPPA. These changes include (1) a fast exponential (FREXP), (2) a two-argument Planck function, and (3) the use of the average opacities from KAPPA (θ and ρ interpolation) for the monofrequency calculation as well as for the Planck opacities.

The new fast exponential routine FREXP uses table lookup and interpolation rather than the normal expansion methods. The routine is written in machine language but uses the library routine EXP(X) for positive X or $X > -10$. An over-all gain in speed of a few percent was achieved in one comparison SPUTTER calculation.

The PLNKUT routine, with its associated tables PLNKTT, has been corrected and made more efficient by using a two-argument call which now calculates from either the analytic form or from the tables the difference in

$$b(u_1, u_2) = \frac{1}{B} \int_{u_1}^{u_2} \frac{h\nu^3}{c^2} \frac{1}{e^{-h\nu/kT} - 1} dv = b_j . \quad (5.6)$$

The accuracy is improved since now not only differences of nearly equal numbers are subtracted.

The subroutine KAPPA, which calls in the group-averaged absorption coefficients from the DIANE tape and performs a bilinear log interpolation in temperature and density, has been modified to obtain the grey absorption coefficients as well as the Planck averages. At present, the format of the DIANE (absorption coefficient) tape includes a BCD record for tape identification, the Rosseland and Planck averages for a selected set of temperatures and densities from 0.25 ev to 50 ev and from 10 normal to 10^{-6} normal, and the actual integration, $\int \kappa_\nu dv$, for the grey case. The grey or frequency-integrated averages are also used for an estimate of the time steps in PRADTN. KAPPA reads in first the tape name, the number of frequency groups, and the size of the records. If the sentinel for multifrequency is set to KMAX = 1, then the first frequency group, $h\nu_1$, and its absorption coefficients are read into storage. The interpolations in $\log \theta_i$ and $\log \rho_i$ are performed and a return to PRADTN is

made. If KMAX = 0, then KAPPA skips over the frequency-dependent absorption coefficients and reads into storage the grey averages. A signal, S15 = 0, is subsequently set, and for further cycles the interpolations are made on the stored quantities; the tape is not called again.

5.5. INPUT NUMBERS

The input quantities used in the radiation-transport subroutines and their functions are listed in Table 5.1. The entries in it are as follows: column 1 is the storage location number used for entering the quantity into storage with the CARDS subroutine, column 2 lists the FORTRAN name of the stored quantity, column 3 gives the range of admissible values of the input quantity, column 4 describes its function and identifies special values it may assume, and column 6 records a set of values of the quantities which might be typical of those for a normal problem. Included is a set of values for the input quantities selected for solving typical problems.

5.6. EDITS

The editing of such frequency-dependent quantities as H3, the optical depth (Rosseland), X6, the source ($b_j \theta^4$), X2, the flux (in ergs/4/3 π sec) X2/DHNU, the flux divided by the frequency group, THETA, the temperature (ev), and EI, the energy (ERGS/G) versus radius is accomplished by setting S12 to the desired number of cycles between prints. These multi-frequency edits have been used to evaluate the criteria for the subroutines as well as for diagnostics during the calculations.

A list of sample editing for a particular frequency group is given on page 27. The HNU is in electron volts. The quantities found useful to display for each frequency group and for a characteristic ray are listed on page 28. The format statements, in the listings appended, have been revised for the debug print from those used on page 28.

Table 5.1
PLANE RADIATION INPUT QUANTITIES

Card No.	Quantity	Range of Values	Description	Typical Value
37	LMDA(37)	2, 3, 4, 5, 6	Number of angles with $\mu > 0$.	2
44	KMAX	----	$\neq 0$, performs multigroup frequency approximation; $= 0$, performs single-group frequency approximation.	0
81	HVB	≥ 0	Number of optical mean free paths by which a transport region is extended at the expense of each adjacent diffusion region. (See Section 3.2.)	5
83	HCB	≥ 0	Criterion to define a diffusion region in terms of relative gradient of the source function. Diffusion regions are eliminated if 0. (See Section 3.2.)	0.1
87	CB	≥ 0	Criterion to combine frequency groups. If the lower frequency of the group is more than CB times the temperature of the hottest zone, that group is combined with the adjacent group of lower frequency. A half-integer value presents termination of the problem when half or more of the groups have been combined. (See Section 5.1.1.)	10.5
88	GA	≥ 0	One of two criteria for choice of linear or stepwise constant source within a zone. (See Section 5.1.2.)	0.333
90	GL	Neg., 0, $\frac{1}{2}$, pos. integer	Indicator for radiation boundary condition at IB. GL = negative, total reflection; GL = 0, intensity for $\mu < 0$ is zero; GL = $\frac{1}{2}$, blackbody intensity based on temperature located in THETA(IB) for $\mu < 0$; GL = positive integer, intensity for $\mu < 0$ obtained from source routine. GL must equal number of frequency groups. (See Section 2.1.3.)	0
121	AC	≥ 0	One of two criteria for choice of linear or stepwise constant source. Minimum value for using a linear source. (See Section 5.1.2.)	0.3
127	AC03T4	----	Transport debug edit criterion. Edit occurs if $\neq 0$ and < cycle number.	9
147	S12	----	Number of cycles between multifrequency edits.	10
150	S15	0, 1	Trigger controlling call of DIANE tape. Must have value $\neq 0$ on starts or restarts.	1
8466	TELM(25)	≥ 0	Constant multiplying the radiation time step. Can be used to modify the stability criterion.	1
8478	TELM(37)	≥ 0	Maximum permissible fractional energy in any zone due to radiation. Time step may be reduced to meet this requirement.	0.05
8858	SOLID(10)	----	Thick-thin criterion. If 0, Planck mean is used to form H2; otherwise, Rosseland mean. (See Section 4.)	1

Table 5.1
SAMPLE EDIT FOR A CHARACTERISTIC DIRECTION FOR PTRANS

FREQUENCY BAND FROM	17,8000	TO	20,10000	ICX =	31	ICK =	31	ICY =	23
1	-7.5994889-08	0.		X6	2.43339197+02	H3		SUMX3	SUMX4
2	9.99999999+00	0.		X6	2.43339192-01	H3	0.	0.	0.
3	1.00100000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
4	1.00200000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
5	1.00300000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
6	1.00400000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
7	1.00500000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
8	1.00600000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
9	1.00700000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
10	1.00800000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
11	1.00900000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
12	1.01000000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
13	1.01100000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
14	1.01200000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
15	1.01300000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
16	1.01400000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
17	1.01500000+01	0.		X6	2.43339192-01	H3	0.	0.	0.
18	1.01600000+01	0.		X6	2.43339191-01	H3	0.	0.	0.
19	1.01700000+01	0.		X6	2.43339191-01	H3	0.	0.	0.
20	1.01800000+01	0.		X6	2.43339191-01	H3	0.	0.	0.
21	1.01900000+01	0.		X6	2.43339191-01	H3	0.	0.	0.
22	1.01999993+01	0.		X6	2.4314869-01	H3	0.	0.	0.
23	1.0209599+01	4.9129211-04		X6	2.4314869-01	H3	0.	0.	0.
24	1.0216361+01	8.7425114+00		X6	2.7366146-03	H3	2.7876050-01	0.	-1.5491000-03
25	1.0219025+01	3.0955258+01		X6	1.7085025-03	H3	1.2072228+01	5.4142551+00	-3.6999020-02
26	1.0219959+01	3.2643747+01		X6	1.6747771-03	H3	1.2082294+01	6.1653042+00	-3.2881306-02
27	1.0220899+01	3.2132795+01		X6	1.6698545-03	H3	1.2048018+01	9.4688165+00	1.4671562-03
28	1.0221636+01	3.1355411+01		X6	1.63997733-03	H3	7.5149186+00	1.1024201+01	1.9501436-02
29	1.0222843+01	3.3102363+01		X6	1.4826168-03	H3	5.7588749+00	1.2424946+01	3.7044026-02
30	1.0223844+01	4.5108789+01		X6	1.0629491-03	H3	3.84779576+00	1.3015454+01	5.5390377-02
31	1.0224930+01	6.0067691+01		X6	7.6399395-04	H3	1.8744850+00	1.5234913+01	7.4245233-02
32	1.0225205+01	0.		X6	0.	H3	1.6622066+01	9.2370485-02	

Table 5.2
SAMPLE MULTIFREQUENCY EDIT FOR PTRANS

CYCLE =	63.	TIME =	0.305089-07	MMU FROM	17.8000 TO	20.1000
1		R	H3	X6	X2	X2/0MMU
1-2.	81013952-01	2.28637834-02	0.	-0.	-0.	0.
2	9.999999888+00	2.28637835-01	0.	-1.005551455+07-4.	71997637+06	0.
3	1.000399999301	2.28637835-01	0.	-1.817483174+07-7.	90346000+06	0.
4	1.001999999+01	2.28637831-01	0.	-3.04437445+07-1.	32364126+07	0.
5	-0.002999999201	2.28637831-01	0.	-5.09894890+07-2.	2166934640+07	0.
6	1.003999998+01	2.28637831-01	0.	-8.158400+07-3.	1373225+07	0.
7	1.004999998+01	2.28637832-01	0.	-1.63122512+08-6.	22271600+07	0.
8	1.005999998+01	2.28637831-01	0.	-2.39907546+08-1.	04307639+08	0.
9	1.006999998+01	2.28637832-01	0.	-4.02371692+08-1.	6346214+08	0.
10	1.007999998+01	2.28637833-01	0.	-6.75427098+08-2.	3663956+08	0.
11	1.008999998+01	2.28637832-01	0.	-8.1520550+08-4.	935474+08	0.
12	1.009999998+01	2.28637833-01	0.	-1.91150912+09-8.	3109036+08	0.
13	-1.00989998401	2.28637831-01	0.	-3.22769322+09-1.	60325794+09	0.
14	1.01190+8601	2.28637831-01	0.	-5.47133190+09-2.	37884900+09	0.
15	-1.01299998401	2.28637831-01	0.	-9.32924769+09-6.	056192642+09	0.
16	1.013999974+01	2.28637831-01	0.	-1.60407653+10-6.	97425459+09	0.
17	1.014999974+01	2.28637829-01	0.	-2.16074358+10-1.	213640210	0.
18	1.015999974+01	2.28637829-01	0.	-4.23469158+10-2.	4551011+10	0.
19	1.016999974+01	2.28637826-01	0.	-8.91642235+10-3.	87670543+10	0.
20	1.01799974+01	2.28637841-01	0.	-1.65617304+11-7.	20075244+10	0.
21	-1.01899974+01	2.28622492-01	0.	-3.18025679+11-1.	38302472+11	0.
22	1.01999871+01	2.19749393-01	0.	-6.36769354+11-2.	76856246+11	0.
23	-1.02093679+01	2.22925232-02	4.91292107-06-1.	-42616681+12-6.	26073837+11	0.
24	1.0215748+01	2.33086449-03	8.66041410+00-8.	-76098961+11-3.	80912599+11	0.
25	1.02179935+01	1.76119059-03	3.10672917+01-6.	-73073798+11-2.	92640784+11	0.
26	1.02187515+01	1.65541358-03	3.27618031+01	-72651330+11-1.	18544058+31	0.
27	1.02198487+01	1.63309816-03	3.22924628+01	-1.52772108+11	6.6224570+10	0.
28	1.02208086+01	1.65173852+01	3.15173852+01	5.69157353+11	2.47459723+11	0.
29	-1.02218024+01	1.51174245-01	3.7228744+01	-2.8719634+11	4.29216072+11	0.
30	1.02228336+01	1.05740126-03	4.51016038+01	1.40871439+12	6.1248+30+11	0.
31	-1.02239041+01	7.44561593-03	6.0000631300+01	1.80893426+12	7.86493161+11	0.
32	1.02251422+01	6.19309597-01	0.	2.16810211+12	9.42653104+11	0.
						0.

SECTION VI
TIMING STUDIES AND ACCURACY IN
ANGULAR INTEGRATION

6. 1. TIMING CALLS

The comparison in calculation time was obtained by using timing calls at selected locations in the logic of the code. To use the timing calls, it was necessary to establish a fiducial time from the system clock and then print the location of the time call, the time, and the difference in time between calls for each call. The subroutine that carries out these steps is CLOCK.

In the calculations described above, the subroutine CLOCK was called at the following locations in PRADTN and PTRANS:

PRADTN

- 13. 105 - Before frequency loop
- 13. 140 - After call KAPPA on merge
- 13. 701 - After call KAPPA on main frequency loop
- 13. 151 - After calculating general sources
- 13. 180 - Before calling PTRANS
- 13. 292 - After EDIT (normal) end of frequency loop
- 13. 286 - After last frequency start time step
- 13. 239 - End of cycle (return to main program)

PTRANS

- 14. 708 - Before debug print

The following calculation was timed in units of 1/60 sec for the above breakdown in computing time.

The calculation described here did not use the TG criteria (see Section 5.1.2) nor the special boundary conditions (see Section 5.2.4). Three ray passes were completed for each frequency group for a total of six angles, forward and back, and with 32 active zones. The total time for 21 frequency groups was ~14.9 sec. The breakdown in time for a

single frequency group (in units of 1/60 sec) are the following:

Call KAPPA for absorption coefficient	14.
After sources	1.
Characteristic ray passes (3)	3.
After call PTRANS with EDIT	23.
Average time required	$\sim 41/hv$
The start and merge of KAPPA is	~ 32
Total time with EDIT	$\sim 869 (1/60 \text{ sec})$
Total time without EDIT	$\sim 515 (1/60 \text{ sec})$

6.2. ACCURACY IN ANGULAR INTEGRATIONS

Comparisons have been made between calculations for two sets of angles for a radiation shock problem. The problem consists of a hot (5 ev) shock moving into cold low-density air. The effect on the flux versus linear zones for a set of four and eight angles is given in Fig. 6.1. This result indicates that as few as six and probably even four angles would be sufficient for reasonable accuracy.

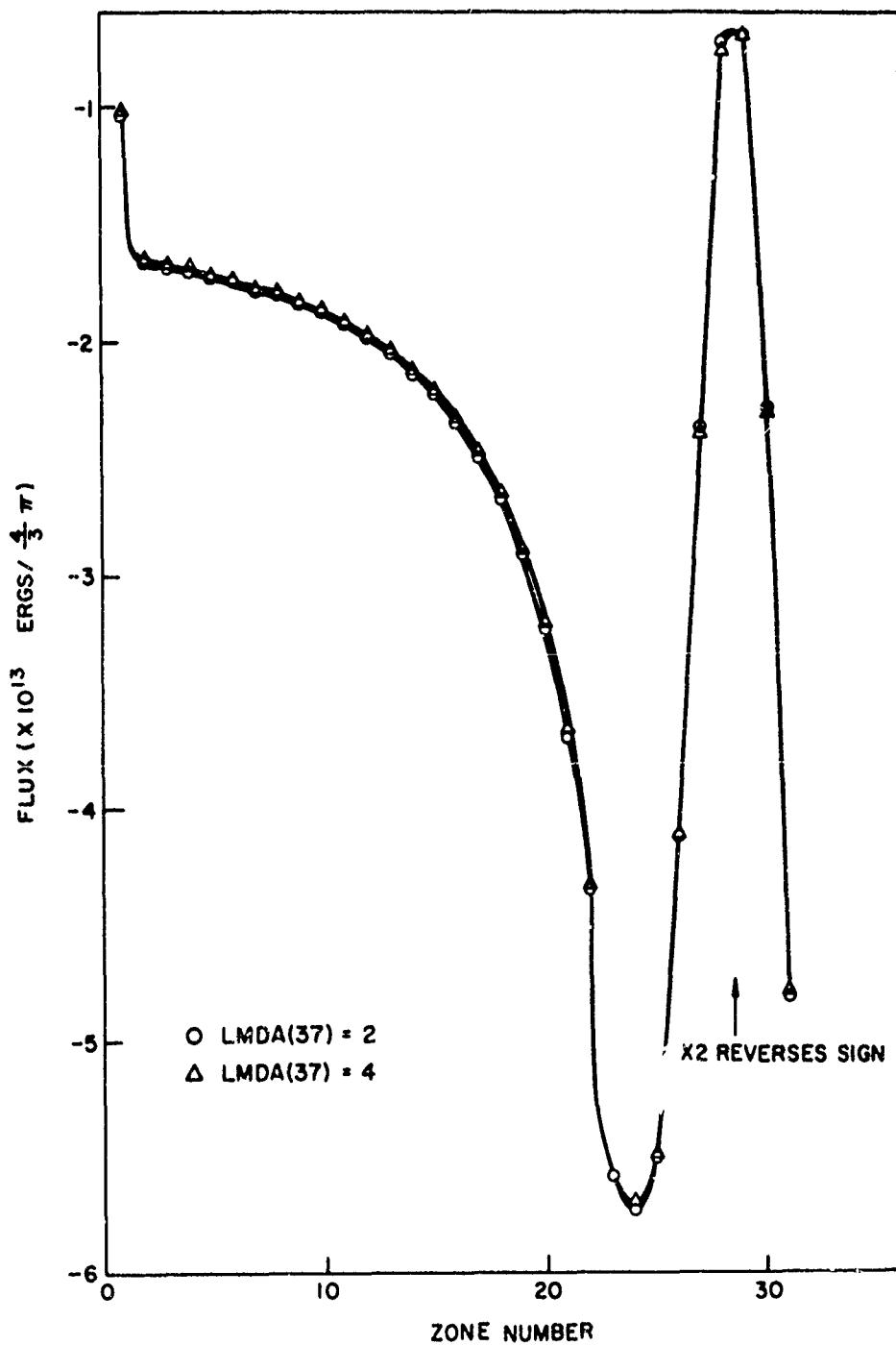


Fig. 6.1--Flux vs linear zones for six and ten angles

REFERENCE

1. Margenall, H., and G. Murphy, The Mathematics of Physics and Chemistry, D. Van Nostrand Co. Inc., New York, 1943.

Appendix A

PRADTN

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SIBFIC PRADTN FULIST,DECK,REF PRAD000
      SUBROUTINE RADTN PRAD001
C COMPILED OCTOBER 7, 1965 WBL
C   PLANE CHARACTERISTIC TRACE WITH DOUBLE GAUSSIAN INTEGRATION PRAD0030
C*****PRAD0040
C*          SPUTTER COMMON **PRAD0050
C*                                     *PRAD0060
C
COMMON LMDA(37), NR , NSMLR , IA , IB , ICA , ICB , PRAD0070
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1 , ISPL , ICAP1 , ICBP1 , PRAD0080
2 II , IG , NRAD , BLANK4, IAM1 , ISMI , ICAM1 , IC8MI , PRAD0090
3 IIP1 , IGM1 , IALPHA, BLANK5, TH , TMAX , BLANK6, DELPRT, PRAD0100
4 FREQ , CNTMAX, AR , ASMLR , PUSHA , PUSHB , BOILA , BOILB , PRAD0110
5 CVA , CVB , SLUG , ALPHA , HVA , HVB , HCA , HCB , PRAD0120
6 EMINA , EMINB , CA , CB , GA , GB , GL , GR , PRAD0130
7 RHOL , RHOR , EPIO , EPSI , RIA , RIB , RDIA , RDIB , PRAD0140
8 RPIA , RPIB , RPDIA , RPDIB , TPRINT, TA , TB , TC , PRAD0150
COMMON TD , TE , DTH2 , DTH2P , DTH1 , DTRMIN, DTMAX , PRAD0160
1 DTMAX1, DTMAX2, DTMAX3, DTR , SWITCH, CO , CMIN , DELTA , PRAD0170
2 GAMA , WCRIT , SIGMAQ, AC , AC03T4, CNVRT , SUMRA , SUMRB , PRAD0180
3 ROIA , ROIAMI, ROIIB , ROI8P1, GMS , S1 , S2 , S3 , PRAD0190
4 S4 , S5 , S6 , S7 , S8 , S9 , S10 , S11 , PRAD0200
5 S12 , S13 , S14 , S15 , S16 , S17 , S18 , S19 , PRAD0210
6 S20 , EO , F0 , TAU , ZERO , R (152), DELTAR(152), PRAD0220
7 ASQ (152), RD (152), VD (152), RDD (152), SMLR (152), PRAD0230
8 DELR ( 37), P (152), P1 (152), PB (152), PB1 (152) PRAD0240
COMMON P2 (152), SV (152), RHO (152), THETA (152), PRAD0250
1 W (152), E (152), EI (152), EK (152), A (152), PRAD0260
2 V (152), G (152), D (152), C (152), X2 (152), PRAD0270
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152), PRAD0280
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152), PRAD0290
5 EC (152), ER (152), SMLQ (152), SMLH (152), BIGA (152), PRAD0300
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152), PRAD0310
7 CHIR (152), CAPAC (152), CAPAR (152), CRTA (152), CRTC (152), PRAD0320
8 CRTPC (152), GOFR (152), FEW (152), CAR (152), OKLM ( 37) PRAD0330
COMMON TELM ( 37), EKLM ( 37), ELM ( 37), FCLM ( 37), PRAD0340
1 FRLM ( 37), WLM ( 37), QLM ( 37), AMASNO( 37), CHRNO ( 37), PRAD0350
2 ZP1 ( 37), ZP2 ( 37), SOLID ( 37), ECHCK ( 37), RK (104), PRAD0360
3 RL ( 37), RHOK (104), ROK (104), THETAK(104), TEMP ( 16), PRAD0370
4 HEAD ( 12), MAXL , MAXLM PRAD0380
C*                                     **PRAD0390
C*****PRAD0400
DIMENSION Q3(1),TG(1),H2(1),Q1(1),X8(1),SUMX3(1),SUMX4(1) PRAD0410
DIMENSION H4(1),Y2(1),H1(1),SUMX2(1),Q2(1) PRAD0420
DIMENSION Q37(1), Q38(1), H3(1) PRAD0430
COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY PRAD0440
COMMON /CNTRL/ SCYCLE, JMULT PRAD0450
COMMON /DAVIS/ ICX, ICY PRAD0460
COMMON /TQ/ QINT1(300), QINT2(300), TITLE(12) PRAD0470
C
EQUIVALENCE(SMLA,H4),(SMLD,Y2) PRAD0490
EQUIVALENCE (BC,TG),(BIGB,H),(CRTA,SUMX2),(CHIC,SUMX3) PRAD0500
EQUIVALENCE (SMLH,X8),(CAR,Q37),(CHIR,Q38),(SMLC,H3) PRAD0510
EQUIVALENCE (AC03T4,TRDBG),(S12,EDITMF) PRAD0520
EQUIVALENCE (EC,Q1),(X7,H2),(BIGA,SUMX4),(GOFR,Q3) PRAD0530
C                                     PRAD0540

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C*****PRAD0550
C*****PRAD0560
C*****PRAD0570
C*****PRAD0580
C*****PRAD0590
C*****PRAD0600
C*****PRAD0610
C*****PRAD0620
C*****PRAD0630
C*****PRAD0640
C*****PRAD0650
C*****PRAD0660
C*****PRAD0670
C*****PRAD0680
C*****PRAD0690
C*****PRAD0700
C*****PRAD0710
C*****PRAD0720
C*****PRAD0730
C*****PRAD0740
C*****PRAD0750
C*****PRAD0760
C*****PRAD0770
C*****PRAD0780
C*****PRAD0790
C*****PRAD0800
C*****PRAD0810
C*****PRAD0820
C*****PRAD0830
C*****PRAD0840
C*****PRAD0850
C*****PRAD0860
C*****PRAD0870
C*****PRAD0880
C*****PRAD0890
C*****PRAD0900
C*****PRAD0910
C*****PRAD0920
C*****PRAD0930
C*****PRAD0940
C*****PRAD0950
C*****PRAD0960

C          EDITMF SAME AS      S12
C          H    SAME AS      BIGB
C          H2 SAME AS X7
C          H3    SAME AS      SHLC
C          H4    SAME AS      SMLA
C          Q1    SAME AS      EC
C          Q3    SAME AS      GQFR
C          Q37   SAME AS      CAR
C          Q38   SAME AS      CHIR
C          SUMX2  SAME AS      CTRR
C          SUMX3  SAME AS      CHIC
C          SUMX4  SAME AS      BIGA
C          TG     SAME AS      BC
C          TRDBG  SAME AS      AC03T4
C          X8     SAME AS      SMLH
C          Y2     SAME AS      SMLD

C          FEX, FM, SUMRHO, CSQD, XSQD, Y, YSQD, Q2, NOT USED

C          PLANES ONLY

C          BOUNDARY CONDITIONS

C          L.H. BLACKBODY IF SOLID ON LEFT

C          NO VAPOR ZONE HAS FLUX OUT FROM SOLID

C          NTIMES=80ILB
C          IM=IBM1
C          IN=IA
C          IF(ZP1(26).EQ.0.) GO TO 15
C          SAVE STUFF FROM EIONX FOR NONEQ AND RESET IN OR IM
C          IF (PUSHA .LT. 0.0) GO TO 100
C          IM = NR - 1
C          WSZ2=BC(IM+1)
C          WSZ3=BR(IM+1)
C          WSZ4 = CRTC(IM+1)
C          WSZ5=RHO(IM+1)
C          GO TO 15
100 IN = NR
C          WSZ2 = BC(IN-1)
C          WSZ3 = BR(IN-1)
C          WSZ4 = CRTC(IN-1)
C          WSZ5 = RHO(IN-1)

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```

15 CONTINUE          PRAD0990
IMP1=IM+1          PRAD1000
INM1=IN-1          PRAD1010
CALL CVCHK (K000FX) PRAD1020
IF (IMP1-IN) 190,190,125 PRAD1030
C
C          NO VAPOR ZONES          PRAD1040
C
C 190 X2(IMP1) = 1.0283E12 * A(IM) * (THETA(IM)**4 - THETA(IMP1)**4) PRAD1070
ER(IM)=-X2(IMP1) PRAD1080
GO TO 1300 PRAD1090
125 IR=IN          PRAD1100
THTAMX=.025        PRAD1110
IF (IALPHA-1) 130,140,130 PRAD1120
130 S1 = 13.0130    PRAD1130
CALL UNCLE        PRAD1140
140 DO 180 I=IN,IM PRAD1150
X3(I)=0.          PRAD1160
X4(I)=0.          PRAD1170
X5(I)=0.          PRAD1180
X6(I)=0.          PRAD1190
CRTR(I)=0.         PRAD1200
C
C          SET UP FOR KAPPA INTERPOLATION          PRAD1210
C
C  Q1(I)=THETA(I)**4          PRAD1220
Q37(I)=ALOG(THETA(I))        PRAD1230
Q38(I)=ALOG(SV(I))          PRAD1240
C
C          FIND IR, RIGHTMOST ZONE WITH THETA GREATER THAN 0.05 EV          PRAD1250
C
C  IF (THETA(I)-THTAMX) 160,160,150          PRAD1260
150 THTAMX=THETA(I)          PRAD1270
160 IF (THETA(I)-0.05) 170,170          PRAD1280
170 IR=I          PRAD1290
180 CONTINUE          PRAD1300
IF (THTAMX .LT. THETA(18)) THTAMX = THETA(18)          PRAD1310
C
C*****          PRAD1320
C
C          B E G I N   F R E Q U E N C Y   L O O P          PRAD1330
C
C*****          PRAD1340
200 HNUP = 3.E3          PRAD1350
C
C          SET UP MAX FREQ BOUNDARY          PRAD1360
C
C  HNUP4 = 8.1E13          PRAD1370
IHN4=1          PRAD1380
DO 210 I=IN,IMP1          PRAD1390
210 SUMX2(I)=0.0          PRAD1400
IF (KMAX.EQ.0) GO TO 280          PRAD1410
C
C          THIS CODING WONT WORK IF HNU NOT EVALUATED          PRAD1420
          PRAD1430
          PRAD1440
          PRAD1450
          PRAD1460
          PRAD1470
          PRAD1480
          PRAD1490
          PRAD1500
          PRAD1510
          PRAD1520
          PRAD1530

```

```

C
220 CALL KAPPA(IN,IM) PRAD1540
HNU4=HNU**4 PRAD1550
DHNUP = DHNU PRAD1560
DHNU = DHNU - HNU 9/29/65
PRAD1570
C
C   MERGE GROUPS WITH HNU MORE THAN CB  TIMES LARGEST THETA PRAD1580
C
C   IF (THTAMX- HNU/CB) 240,300,300 PRAD1590
C
C           REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE PRAD1600
C
C   240 IF (IHNU+IHNU-NHNU) 260,250,250 PRAD1610
250 IF (AMOD(CB,1.) .EQ. 0.5) GO TO 260 PRAD1620
S1=13.0250 PRAD1630
CALL UNCLE PRAD1640
260 DO 270 I=IN,IM PRAD1650
BETA=HNU/THETA(I) PRAD1660
BETAP=HNUP/THETA(I) PRAD1670
DFB=PLNKUT(BETA,BETAP) PRAD1680
IF (DFB.EQ.0.) GO TO 270 PRAD1690
TEMP(1)=DFB*Q1(I) PRAD1700
EMB1=EXP(-BETA) PRAD1710
EMB2=EXP(-BETAP) PRAD1720
TEMP(2)=DFB+0.0384974/Q1(I)*(HNU4/(1.0-EMB1) PRAD1730
1*EMB1-HNUP4/(1.0-EMB2)*EMB2) PRAD1740
PRAD1750
PRAD1760
PRAD1770
PRAD1780
PRAD1790
C
C           FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS PRAD1800
C
C   X6(I)=X6(I)+TEMP(1) PRAD1810
X4(I)=X4(I)+TEMP(2) PRAD1820
X5(I)=X5(I)+CAPAC(I)*TEMP(1) PRAD1830
X3(I)=X3(I)+TEMP(2)/CAPAR(I) PRAD1840
PRAD1850
270 CONTINUE PRAD1860
IF (GL .LT. 1. .OR. IHNU .EQ. 1) GO TO 275 9/29/65
C
C   MERGE FREQUENCY-DEPENDENT EXTERNAL INPUT INTENSITIES PRAD1880
NHNU = LMDA(37) PRAD1890
IHNU = NMU * (IHNU - 2) 9/29/65
DO 272 I = 1, NMU PRAD1910
IQNT1 = IQNT + I PRAD1920
IQNT2 = IQNT1 + NMU PRAD1930
IFI(IHNU.GT.2) DHNUP=1. 9/29/65
272 QINT1(IQNT2) = QINT1(IQNT2)*DHNU + QINT1(IQNT1)*DHNU 9/29/65
275 HNUP=HNU PRAD1950
IHNU=IHNU+1 PRAD1960
HNUP4=HNU4 PRAD1970
IF (THTAMX- HNU/CB) 220,310,310 PRAD1980
C
C           MONOFREQUENCY CALCULATION PRAD1990
C
C   280 NHNU=1 PRAD2000
CALL KAPPA (IN,IM) PRAD2010
DO 290 I=IN,IM PRAD2020
X5(I)=1. PRAD2030
290 X6(I)=Q1(I) PRAD2040
PRAD2050
PRAD2060

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```

DFB=1.0
HNU = .001
ICX=IR
IF (GL .GT. 0.0) ICX = IM
ICY=IN
GO TO 480
300 IF (IHNU-1) 550,370,260
C
C          FORM MERGED KAPPAS
C
310 DC 350 I=IN,IM
IF (X6(I)) 320,350,330
320 S1=13.0320
CALL UNCLE
330 CAPAR(I)=X4(I)/X3(I)
340 CAPAC(I)=X5(I)/X6(I)
350 CONTINUE
HNUP = 3.E3
HNUP4 = 8.1E13
DHNU = HNUP - HNU
IHNU=IHNU-1
IF(GL.LT.1.) GO TO 370
DO 355 I=1,NMU
IQNT2 = IQNT + I + NMU
355 QINT1(IQNT2) = QINT1(IQNT2)/DHNU
GO TO 370
C
C          TYPICAL GROUP CALCULATION OF SOURCES
C
360 CALL KAPPA(IN,IM)
DHNU=HNUP-HNU
HNU4=HNU**4
370 IF (GL-1.) 390,380,380
380 IF (HNU.NE.ROK(IHNU+52)) GO TO 490
IF (GL.NE.FLOAT(NHNU)) GO TO 490
C A L C U L A T E   I C X ,   I C Y
390 ICX=IN
ICY = IN
IF (GL .LE. 0.) GO TO 395
ICX = IM
DO 392 I = IN, IM
DFB = PLNKUT(HNU / THETA(I), HNUP / THETA(I))
392 X6(I)=DFB*Q1(I)
GO TO 480
395 DO 470 I=IN,IR
BETA=HNU/THETA(I)
C
C          AVOID CALCULATION OF DFB LESS THAN 1E-5
C
400 IF (BETA-19.0) 400,410,410
400 BETAP=HNUP/THETA(I)
EMB2=EXP(-BETAP)
IF (BETAP-0.01) 410,410,460
410 IF (ICX-IR) 430,420,420
420 ICX=I-

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430 IF (I-ICY) 440,440,450 PRAD2570
440 ICY=ICY+1 PRAD2580
C PRAD2590
C ICX IS INDEX OF LAST ZONE WITH SIGNIFICANT SOURCE PRAD2600
C ICY IS INDEX OF FIRST ZONE WITH SIGNIFICANT SOURCE PRAD2610
C PRAD2620
C PRAD2630
450 X6(I)=0.0 PRAD2640
X5(I)=0.0 PRAD2650
GO TO 470 PRAD2660
C PRAD2670
C FORM SOURCES X6 AND X5 PRAD2680
C PRAD2690
460 DFB=PLNKUT(BETA,BETAP) PRAD2700
X6(I)=DFB*Q1(I) PRAD2710
C TEMP(2)=0.0384974/Q1(I)*(HNU4/(EXP(BETA)-1.0) PRAD2720
C 1 -HNU4/4/(1.0-EMB2)*EMB2) PRAD2730
C X5(I)=DFB*TEMP(2) PRAD2740
ICX=IR PRAD2750
470 CONTINUE PRAD2760
480 IF (INM1) 490,520,500 PRAD2770
C PRAD2780
C SET BLACKBODY CONDITION FOR IA GREATER THAN 1 PRAD2790
C PRAD2800
490 S1=13.0490 PRAD2810
CALL UNCLE PRAD2820
500 DFB = PLNKUT (HNU/THETA(INM1),HNUP/THETA(INM1)) PRAD2830
X6(INM1) = DFB * THETA(INM1)**4 PRAD2840
C SET BLACKBODY CONDITION IF DESIRED FOR IMP1 PRAD2850
520 IF (GL.NE.0.5) GO TO 530 PRAD2860
DFB = PLNKUT(HNU / THETA(IMP1), HNUP / THETA(IMP1)) PRAD2870
X6(IMP1) = DFB * THETA(IMP1)**4 PRAD2880
530 Q31=0.0 PRAD2890
C PRAD2900
C FORM ROSELAND AND PLANCK OPTICAL DEPTHS PRAD2910
C PRAD2920
DO 590 I=IN,IM PRAD2930
IF (CAPAR(I)) 550,550,540 PRAD2940
540 IF (CAPAC(I)) 550,550,560 PRAD2950
550 S1=13.0550 PRAD2960
CALL UNCLE PRAD2970
C PRAD2980
C CHOOSE ALL ROSELAND IF SOLID 10 IS POSITIVE PRAD2990
C PRAD3000
560 IF (SOLID(10).EQ.0.) GO TO 570 PRAD3010
H(I)=CAPAR(I)/SV(I) PRAD3020
GO TO 580 PRAD3030
570 H(I)=CAPAC(I)/SV(I) PRAD3040
580 H2(I)=H(I)*DELTAR(I) PRAD3050
IF (ALPHA .GT. 1.) GO TO 586 PRAD3060
H3(I) = CAPAR(I) * G(I) PRAD3070
GO TO 588 PRAD3080
C AVEAT. ASYNCHRONISMS IN SV AND DELTAR LEAD TO ERRONEOUS FLUCTUATIONS PRAD3090
C IN H3. THIS CAN BE FIXED BY SUBSTITUTING G IN PLANES, BUT SPHERESPRAD3100
C WILL STILL HAVE THIS TROUBLE. PRAD3110

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586 H3(I)=CAPAR(I)/SV(I)*DELTAR(I) PRAD3120
588 Q3I=Q3I+H3(I) PRAD3130
      Q3(I+1)=Q3I PRAD3140
      H(I)=0.5*H(I) PRAD3150
      H2(I)=0.5*H2(I) PRAD3160
      H3(I)=0.5*H3(I) PRAD3170
C PRAD3180
C      ZERO DIFFUSUIN INDICATORS AND X2 PRAD3190
C
      X2(I)=0.0 PRAD3200
      X3(I)=0.0 PRAD3210
      X4(I)=0.0 PRAD3220
590 RHG(I)=0.0 PRAD3230
      X2(IMP1)=0.0 PRAD3240
      X3(IMP1)=0.0 PRAD3250
      X4(IMP1)=0.0 PRAD3260
      IF (ICY .GT. ICX) GO TO 990 PRAD3270
C PRAD3280
C      STEP-LINEAR CRITERION AT ICY PRAD3290
C      UNCONDITIONAL STEP AS BOUNDARY CONDITION IF ICY = IN PRAD3300
C
      IF ((ICY-IN) 675,600,610 PRAD3310
600 Y2(IN)=X6(IN) PRAD3320
      TG(IN)=0.0 PRAD3330
      GO TO 620 PRAD3340
610 TEMP(1)=H3(ICY-1)+H3(ICY) PRAD3350
      TG(ICY)=X6(ICY)/TEMP(1) PRAD3360
      Y2(ICY)=TG(ICY)*H3(ICY-1) PRAD3370
C PRAD3380
C      FORM Y2 AND TG SET X3=-1 IF A DIFFUSION CRITERION MET USING HCB PRAD3390
C
620 ICXM1=ICX-1 PRAD3400
      IF (ICY .GT. ICXM1) GO TO 672 PRAD3410
      DO 670 I=ICY,ICXM1 PRAD3420
      TEMP(1)=H3(I+1)+H3(I) PRAD3430
      IF (AMAX1(X6(I), X6(I+1)) .LE. 0.) GO TO 640 PRAD3440
      IF (AMIN1(H3(I), H3(I+1)) .GT. AC) GO TO 650 PRAD3450
      IF (ABS((H3(I)-H3(I+1))/TEMP(1)) .GT. GA) GO TO 640 PRAD3460
      IF (ABS((X6(I)-X6(I+1))/(X6(I)+X6(I+1)))-GA) 650,650,640 PRAD3470
640 TG(I+1)=0.0 PRAD3490
      GO TO 670 PRAD3500
650 TG(I+1)=(X6(I+1)-X6(I))/TEMP(1) PRAD3510
C PRAD3520
C      TG(I+1)=(Q1(I+1)-Q1(I))/TEMP(1)*(X5(I+1)+X5(I))/2.0 PRAD3530
C
      Y2(I+1)=(X6(I+1)*H3(I)+X6(I)*H3(I+1))/TEMP(1) PRAD3540
      IF (ABS(TG(I+1))-HCB*Y2(I+1)) 660,670,670 PRAD3550
660 X3(I+1)=-1.0 PRAD3560
670 CONTINUE PRAD3570
C PRAD3580
C      RADIATION BOUNDARY CONDITION AT ICX PRAD3590
C      (VACUUM IF ICX = IM AND GL NOT 1/2) PRAD3600
C
672 IF ((ICX-IM) 680,690,675 PRAD3610
675 S1 = 13.0675 PRAD3620
C PRAD3630
C
C PRAD3640
C
C PRAD3650
C
C PRAD3660

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CALL UNCLE
680 TEMP(1)=H3(ICX+1)+H3(ICX) PRAD3670
TG(ICX+1)=-X6(ICX)/TEMP(1) PRAD3680
Y2(ICX+1)=-TG(ICX+1)*H3(ICX+1) PRAD3690
GO TO 700 PRAD3700
690 IF (GL.EQ. 0.5) GO TO 700 PRAD3710
Y2(IMP1)=X6(ICX) PRAD3720
TG(IMP1)=0.0 PRAD3730
PRAD3740
PRAD3750
PRAD3760
PRAD3770
PRAD3780
PRAD3790
PRAD3800
PRAD3810
PRAD3820
PRAD3830
PRAD3840
PRAD3850
PRAD3860
PRAD3870
PRAD3880
PRAD3890
PRAD3900
PRAD3910
PRAD3920
PRAD3930
PRAD3940
PRAD3950
PRAD3960
PRAD3970
PRAD3980
PRAD3990
PRAD4010
PRAD4020
PRAD4030
PRAD4040
PRAD4050
PRAD4070
PRAD4080
PRAD4090
PRAD4100
PRAD4110
PRAD4120
PRAD4130
PRAD4140
PRAD4150
PRAD4160
PRAD4170
PRAD4190
PRAD4200
PRAD4210

C EXTEND TRANSPORT REGION BOUNDARIES, IF NEEDED, TO PROVIDE HVB MEAN
C FREE PATHS
C
700 I=IN+1
710 IF (X3(I)) 720,740,730
720 I=I+1
IF (I-ICX-1) 710,740,820
730 S1=13.0730
CALL UNCLE
740 J=I-1
750 IF (Q3(I)-Q3(J)-HVB) 760,760,770
760 X4(J)=-1.0
J=J-1
IF (J-IN) 770,750,750
770 I=I+1
IF (I-ICX-1) 780,780,820
780 IF (X3(I)) 790,770,730
790 J=I
800 IF (Q3(J)-Q3(I-1)-HVB) 810,810,720
810 X4(J)=-1.0
J=J+1
IF (J-ICX-1) 800,720,720
820 I=IN+1

C TEST TO FORM TRANSPORT REGIONS
C
830 IAX=IN
840 IF (X3(I)) 850,860,730
850 IF (X4(I)) 860,870,730
C
C REMOVE ONE ZONE DIFFUSION REGION
C
860 I=I+1
IF (I-ICX-1) 840,950,950
870 I=I+1
IF (I-ICX-1) 890,950,950
880 If (X3(I)) 890,840,730
890 I. X4(I)) 840,900,730
:00 IP =I-3
GO TO 960
910 IF (X3(I)) 920,940,730
920 IF (X4(I)) 940,930,730
C FORM X2 FOR DIFFUSION ZONES IN ORDER
930 X2(I) = -1.37E12 * TG(I)
I=I+1
IF (I ICX-1) 910,980,980

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C
      WSB = 0.0          PRAD4760
      DO 1075 I = 1, MAXLM PRAD4770
1075 WSB = WSB + ELM(I) PRAD4780
      DTR1=1.E10          PRAD4790
      DTR2=1.E10          PRAD4800
      IF (KMAX.EQ.0) GO TO 1080 PRAD4810
      CALL KAPPA(IN,IM)    PRAD4820
1080 DO 1230 I=IN,IM    PRAD4830
C
C           IF ROSS IS ZERO EXIT
C
      IF (CAPAR(I)) 1090,1090,1100 PRAD4840
1090 S1=13.1090          PRAD4850
      CALL UNCLE          PRAD4860
1100 TEMP(3)=CAPAR(I)    PRAD4870
      IF (SCLID(10)) 1110,1120,1110 PRAD4880
1110 TEMP(1)=CAPAR(:)    PRAD4890
      GO TO 1130          PRAD4900
1120 TEMP(1)=SQRT(CAPAR(I)*CAPAC(I)) PRAD4910
1130 IF (TEMP(1)) 1090,1090,1140 PRAD4920
1140 H(I)=0.5*TEMP(1)/SV(I)    PRAD4930
      H3(I) = H(I) * DELTAR(I) PRAD4940
      IF (.001-THETA(I)) 1160,1230,1230 PRAD4950
1160 IF (H3(I).GT.0.1) GO TO 1170 PRAD4960
      IF (ER(I).EQ.0.) GO TO 1170 PRAD4970
      WSB8 = E(I) * G(I)    PRAD4980
      IF (TELM(37) .EQ. 0.0) GO TO 1170 PRAD4990
      IF (WSB8 - TELM(37) * WSB) 1170, 1165, 1165 PRAD5000
1165 TEMP(2)=.5*CV(I)*THETA(I)*G(I)/ABS(ER(I)) PRAD5010
      GO TO 1180          PRAD5020
1170 TEMP(2)=(.5+1.5*H3(:)**2)*CV(I)/(4.1132E12*TEMP(3)*THETA(:)**3) PRAD5030
      TEMP(2)=TEMP(2)*TELM(25) PRAD5040
***** *PRAD5050
C
C           F I N D   M I N I M U M   T I M E   S T E P
C
***** *PRAD5060
1180 IF (TEMP(2)) 1230,1230,1190 PRAD5070
1190 CONTINUE          PRAD5080
      IF (TEMP(2)-DTR1) 1200,1210,1210 PRAD5090
1200 DTR2=DTR1          *PRAD5100
      IMN2=IMN1          *PRAD5110
      DTR1=TEMP(2)        *PRAD5120
      IMN1=I              PRAD5130
      GO TO 1230          PRAD5140
1210 IF (TEMP(2)-DTR2) 1220,1230,1230 PRAD5150
1220 DTR2=TEMP(2)        PRAD5160
      IMN2=I              PRAD5170
1230 CONTINUE          PRAD5180
      DTRMIN=DTR1        PRAD5190
      EO=IMN1            PRAD5200
C
C           P R I N T   M I N I M U M   T I M E   S T E P S   B E T W E E N   E D I T S
C
      PRAD5210
      PRAD5220
      PRAD5230
      PRAD5240
      PRAD5250
      PRAD5260
      PRAD5270
      PRAD5280
      PRAD5290
      PRAD5300

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Appendix B
PTRANS

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$IBFTC PTRANS FULIST,DECK,REF
      SUBROUTINE TRANS(N,M)                                         PTRAO000
C      CCOMPILED JULY 1, 1965  WBL                                         PTRAO010
C      PLANE CHARACTERISTIC TRACE WITH DOUBLE GAUSSIAN INTEGRATION      PTRAO020
C      DECK DBLGAU REQUIRED FOR INTEGRATION COEFFS.                      PTRAO030
C*****PTRAO050
C*          S P U T T E R   C O M M O N                               **PTRAO060
C*                                                               *PTRAO070
C
COMMON  LMDA(37), NR      , NSMLR , IA      , IB      , ICA      , ICB      , PTRAO080
1      KMAX      , BLANK1, BLANK2, BLANK3, IAP1      , IBP1      , ICAP1      , IC8P1      , PTRAO090
2      II       , IG      , NRAD      , BLANK4, IAM1      , IBM1      , ICAM1      , ICBM1      , PTRAO100
3      IIP1      , IGM1      , IALPHA, BLANK5, TH      , TMAX      , BLANK6, DELPRT, PTRAO110
4      FREQ      , CNTMAX, AR      , ASMLR , PUSHA , PUSHB , BOILA , BOILB , PTRAO120
5      CVA       , CVB      , SLUG      , ALPHA , HVA      , HVB      , HCA      , HCB      , PTRAO130
6      EMINA    , EMINB    , CA      , CB      , GA      , GB      , GL      , GR      , PTRAO140
7      RHCL      , RHOR      , EPIO      , EPSI , RIA      , RIB      , RDIA      , RDI8      , PTRAO150
8      RPIA      , RPIB      , RPDIA , RPDIB , TPRINT, TA      , TB      , TC      , PTRAO160
COMMON  TD      , TE      , DTH2      , DTH2P , DTH1      , DTRMIN, DTMAX , PTRAO170
1      DTMAX1, DTMAX2, DTMAX3, DTR      , SWITCH, CO      , CMIN      , DELTA , PTRAO180
2      GAMA      , WCRIT , SIGMAQ, AC      , AC03T4, CNVRT , SUMRA , SUMRB , PTRAO190
3      ROI A    , ROIAM1, ROI B   , ROI B P1, GMS      , S1      , S2      , S3      , PTRAO200
4      S4       , S5      , S6      , S7      , S8      , S9      , S10     , S11     , PTRAO210
5      S12     , S13     , S14     , S15     , S16     , S17     , S18     , S19     , PTRAO220
6      S20     , EO      , FO      , TAU      , ZERO      , R      , (152), DELTAR(152), PTRAO230
7      ASQ (152), RD (152), VD (152), RDD (152), SMLR (152), PTRAO240
8      DELR (37), P (152), P1 (152), PB (152), PB1 (152), PTRAO250
COMMON  P2 (152), SV (152), RHO (152), THETA (152), PTRAO260
1      W (152), E (152), EI (152), EK (152), A (152), PTRAO270
2      V (152), G (152), D (152), C (152), X2 (152), PTRAO280
3      X3 (152), X4 (152), X5 (152), X6 (152), X7 (152), PTRAO290
4      SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152), PTRAO300
5      EC (152), ER (152), SMLQ (152), SMLH (152), BIGA (152), PTRAO310
6      BIGB (152), CV (152), BC (152), BR (152), CHIC (152), PTRAO320
7      CHIR (152), CAPAC (152), CAPAR (152), CRT C (152), CRT R (152), PTRAO330
8      CRTPC (152), GOF R (152), FEW (152), CAR (152), OKLM (37), PTRAO340
COMMON  TELM (37), EKLM (37), ELM (37), FCLM (37), PTRAO350
1      FRLM (37), WLM (37), QLM (37), AMASNO(37), CHRNO (37), PTRAO360
2      ZP1 (37), ZP2 (37), SOLID (37), ECHCK (37), RK (104), PTRAO370
3      RL (37), RHOK (104), ROK (104), THETAK(104), TEMP (16), PTRAO380
4      HEAD (12), MAXL      , MAXLM      , PTRAO390
C*                                                               **PTRAO400
C*****PTRAO410
DIMENSION Q3(1),TG(1),H2(1),Q1(1),X8(1),SUMX3(1),SUMX4(1)      PTRAO420
DIMENSION H4(1),Y2(1),H1(1),SUMX2(1),Q2(1)                      PTRAO430
DIMENSION Q37(1), Q38(1), H3(1)                      PTRAO440
COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY      PTRAO450
COMMON /CNTRL/ SCYCLE, JMULT                               PTRAO460
COMMON /DAVIS/ ICX, ICY                               PTRAO470
COMMON /TQ/ QINT1(300), QINT2(300), TITLE(12)      PTRAO480
EQUIVALENCE (SMLA,H4),(SMLD,Y2)                      PTRAO490
EQUIVALENCE (BC,TG),(BIGB,H),(CRT C,SUMX2),(CHIC,SUMX3)      PTRAO500
EQUIVALENCE (SMLH,X8),(CAR,Q37),(CHIR,Q38),(SMLC,H3)      PTRAO510
EQUIVALENCE (AC03T4,TRD8G),(S12,EDITMF)                  PTRAO520
EQUIVALENCE (EC,Q1),(X7,H2),(BIGA,SUMX4),(GOF R,Q3)      PTRAO530
C*****PTRAO540

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DIMENSION RR(40)                                PTRAO550
DATA RR/2.113248E-01,7.886752E-01,1.056624E-01,3.943376E-01,
1      1.127017E-01,5.000000E-01,8.872983E-01,3.130600E-02,
2      2.222222E-01,2.464718E-01,6.943180E-02,3.300095E-01,
3      6.699905E-01,9.305682E-01,1.207610E-02,1.076071E-01,
4      2.184655E-01,1.618513E-01,4.691010E-02,2.307653E-01,
5      5.000000E-01,7.692347E-01,9.530899E-01,5.557100E-03,
6      5.522540E-02,1.422222E-01,1.840889E-01,1.129063E-01,
7      3.376520E-02,1.693953E-01,3.806903E-01,6.193096E-01,
8      8.306047E-01,9.662348E-01,2.892400E-03,3.055570E-02,
9      8.906520E-02,1.448918E-01,1.498251E-01,8.276980E-02/   PTRAO650
*PTRAO660
C
C          EDITMF SAME AS      S12
C          H      SAME AS      BIGB
C          H2     SAME AS      X7
C          H3     SAME AS      SMLC
C          H4     SAME AS      SMLA
C          Q1     SAME AS      EC
C          Q3     SAME AS      GOFR
C          Q37    SAME AS      CAR
C          Q38    SAME AS      CHIR
C          SUMX2   SAME AS      CRTR
C          SUMX3   SAME AS      CHIC
C          SUMX4   SAME AS      BIGA
C          TG      SAME AS      BC
C          1RDBG   SAME AS      AC03T4
C          X8      SAME AS      SMLH
C          Y2      SAME AS      SMLD
*PTRAO670
*PTRAO680
PTRAO690
*PTRAO700
*PTRAO710
*PTRAO720
*PTRAO730
*PTRAO740
*PTRAO750
*PTRAO760
*PTRAO770
*PTRAO780
*PTRAO790
*PTRAO800
*PTRAO810
*PTRAO820
*PTRAO830
*****PTRAO840
PTRAO850
PTRAO860
PTRAO870
PTRAO880
PTRAO890
*****PTRAO900
*PTRAO910
*PTRAO920
*PTRAO930
*****PTRAO940
PTRAO950
PTRAO960
PTRAO970
PTRAO980
PTRAO990
PTRAO1000
PTRAO1010
PTRAO1020
PTRAO1030
PTRAO1040
PTRAO1050
PTRAO1060
PTRAO1070
PTRAO1080
PTRAO1090
C
C          FEX, FM, SUMRHO, CSQD, XSQD, Y, YSQD, Q2, NOT USED
C
C          PLANES ONLY
C
C          IAX=N
C          IBX=M
C          IN=IA
C          INM1=IN-1
C          IMP1 = IM + 1
C          CALL DVCHK(K000FX)
C          GO TO (100,110), K000FX
100  S1=14.0100
          CALL UNCLE
110  IBXP1=IBX+1
          IALPHA=ALPHA
C
C          ERROR IF NOT PLANE
C
C          GO TO (130,120,120), IALPHA

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120 S1=14.0120 PTRA1100
CALL UNCLE PTRA1110
130 NY = LMDO(37) - 1 PTRA1120
NMU = (NY - 1) * (NY + 2) + 1 PTRA1130
NGS = NMU + NY + 1 PTRA1140
JJ = 0 PTRA1150
C PTRA1160
C DO POSITIVE ANGLES FIRST PTRA1170
C PTRA1180
140 I=IAX PTRA1190
F2=0.0 PTRA1200
C PTRA1210
C IF IAX=IN TRANSFER TO 150 TO SET SPECIAL BOUNDARY CONDITIONS PTRA1220
C PTRA1230
C IF (IAX-IN) 360,150,180 PTRA1240
C PTRA1250
C CALCULATE BOUNDARY SOURCE INTENSITY PTRA1260
C PTRA1270
150 IF (INM1) 160,310,170 PTRA1280
C PTRA1290
C SET BLACKBODY CONDITION FOR PUSHER PTRA1300
C PTRA1310
160 S1=14.0160 PTRA1320
CALL UNCLE PTRA1330
170 F2=X6(INM1) PTRA1340
GO TO 310 PTRA1350
C PTRA1360
C DIFFUSION BOUNDARY CONDITION AT IAX PTRA1370
C PTRA1380
180 IF (TG(I) .EQ. 0.) Y2(I) = X6(I-1) PTRA1390
TEMP(I)=H2(I-1)/RR(NMU)
X8(I)=TG(I)*RR(NMU)
IF (TEMP(I)-1.E-2) 190,190,200 PTRA1400
PTRA1410
190 F2X = Y2(I-1) - TG(I-1) * RR(NMU) PTRA1420
F2 = ((Y2(I) + Y2(I-1)) * 0.5 + X6(I-1) - F2X-F2) * TEMP(I) + F2X PTRA1430
PTRA1440
GO TO 250 PTRA1450
200 H4(I-1)=FREXP(-TEMP(I)) PTRA1460
F2=Y2(I)-X8(I)+(X8(I)-RR(NMU)*TG(I-1))*H4(I-1) PTRA1470
PTRA1480
GO TO 250 PTRA1490
210 IF (TG(I-1) .EQ. 0.) Y2(I-1) = X6(I-1) PTRA1500
X8(I-1)=TG(I-1)*RR(NMU) PTRA1510
C PTRA1520
C REGULAR INTEGRATION STEP FOR F2, POSITIVE MU PTRA1530
C PTRA1540
220 IF (TG(I) .EQ. 0.) Y2(I) = X6(I-1) PTRA1550
X8(I)=TG(I)*RR(NMU)
TEMP(I)=H2(I-1)/RR(NMU)
IF (TEMP(I)-1.E-2) 230,230,240 PTRA1560
PTRA1570
230 F2 = ((Y2(I) + Y2(I-1)) * 0.5 + X6(I-1) - F2 - F2) * TEMP(I) + F2 PTRA1580
PTRA1590
GO TO 250
240 H4(I-1)=FREXP(-TEMP(I)) PTRA1600
F2=Y2(I)-X8(I)+(F2-Y2(I-1)+X8(I-1))*H4(I-1) PTRA1610
PTRA1620
1+X8(I)-X8(I-1), I-1
250 IF (F2.LT.0.0) GO TO 280 PTRA1630
260 SUMX3(I)=F2 PTRA1640

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IF (TG(I) .EQ. 0.) Y2(I) = X6(I)          PTRAI650
I=I+1                                     PTRAI660
IF (I-IBXP1) 270,270,320                  PTRAI670
270 IF (I-ICX-1) 220,220,290              PTRAI680
C
C           NEGATIVE F2 ERROR
C
280 SI=14.0280                           PTRAI690
CALL UNCLE                                PTRAI700
C
C           NO SOURCE IN ZONE GREATER THAN ICX
C
290 IF (F2.EQ.0.0) GO TO 260              PTRAI710
TEMP(I)=H2(I-1)/RR(NMU)
H4(I-1)=FREXP(-TEMP(I)-TEMP(I))
F2=F2*H4(I-1)
GO TO 260
300 IF (F2.EQ.0.0) GO TO 310              PTRAI720
TEMP(I)=H2(I-1)/RR(NMU)
H4(I-1)=FREXP(-TEMP(I)-TEMP(I))
F2=F2*H4(I-1)
310 SUMX3(I) = F2
I=I+1
IF (I-ICY) 300,300,210                  PTRAI730
C
C           DO NEGATIVE ANGLES SECOND
C
320 I=IBXP1
IF (IBX-IM) 370,330,360                  PTRAI740
330 IF (GL) 480,520,340                  PTRAI750
C   GL = 1/2 MEANS BLACKBODY CONDITION SET AT IMPI
C   GL = POSITIVE INTEGER MEANS INTENSITIES FROM QINT1 TABLE AT IMPI
C   GL = 0 MEANS VACUUM AT IMPI
C   GL NEGATIVE MEANS REFLECTIVE CONDITION AT IMPI
340 IF (GL.NE.0.5) GO TO 350              PTRAI760
F2 = X6(IMPI)
GO TO 480
350 IQNT = JJ + 1 + (NY + 1) * (IHNU - 1)
F2 = QINT1(IQNT) / 68.5 * DHNU
GC TO 480
C
C           ERROR IF INDEX EXCEEDS NORMAL RANGE
C
360 SI=14.0360                           PTRAI770
CALL UNCLE                                PTRAI780
C
C           DIFFUSION BOUNDARY CONDITION AT IBXP1
C
370 IF (TG(I) .EQ. 0.) Y2(I) = X6(I)          PTRAI790
TEMP(I)=H2(I)/RR(NMU)
IF (TEMP(I)-1.E-2) 380,380,390          PTRAI800
380 F2X = Y2(I+1) + TG(I+1) * RR(NMU)
F2 = ((Y2(I) + Y2(I+1)) * 0.5 + X6(I) - F2X - F2X) * TEMP(I) + F2X
GO TO 430
390 H4(I)=FREXP(-TEMP(I))                  PTRAI810

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      F2=Y2(I)+X8(I)+(RR(NMU)*TG(I+1)-X8(I))*H4(I)          PTR2200
      GO TO 430                                                 PTR2210
  399 IF (TG(I+1) .EQ. 0.) Y2(I+1) = X6(I)                  PTR2220
C          REGULAR INTEGRATION STEP FOR F2, NEGATIVE MU        PTR2230
C
  400 IF (TG(I) .EQ. 0.) Y2(I) = X6(I)                      PTR2240
      TEMP(1)=H2(I)/RR(NMU)                                 PTR2250
      IF (TEMP(1)-1.E-2) 410,410,420                         PTR2260
  410 F2 = ((Y2(I) + Y2(I+1)) * 0.5 + X6(I) - F2 - F2) * TEMP(1) + F2  PTR2270
      GO TO 430                                                 PTR2280
  420 F2=Y2(I)+X8(I)+((F2-Y2(I+1)-X8(I+1))*H4(I)+X8(I+1)-X8(I))*H4(I)  PTR2290
  430 IF (F2.LT.0.) GO TO 460                                PTR2300
  440 SUMX4(I)=F2                                         PTR2310
C          FORM CONTRIBUTION TO X2                           PTR2320
C
      X2(I)=X2(I)-(F2-SUMX3(I))*RR(NGS)                   PTR2330
C          RHO(I)=RHO(I)+(F2+SUMX3(I))*RR(NGS)/RR(NMU)    PTR2340
C
      IF (TG(I) .EQ. 0.) Y2(I) = X6(I-1)                  PTR2350
      I=I-1                                                 PTR2360
      IF (I-IA) 530,450,450                                PTR2370
  450 IF (I-ICY) 500,400,400                                PTR2380
  460 S1=14.0460                                         PTR2390
      CALL UNCLE                                         PTR2400
C          NO SOURCE IN ZONE LESS THAN ICY                  PTR2410
C
  470 IF (F2.EQ.0.0) GO TO 480                           PTR2420
      TEMP(1)=H2(I)/RR(NMU)                                 PTR2430
      H4(I)=FREXP(-TEMP(1)-TEMP(1))                         PTR2440
      F2=F2*H4(I)                                         PTR2450
  480 SUMX4(I)=F2                                         PTR2460
  490 X2(I)=X2(I)-(F2-SUMX3(I))*RR(NGS)                   PTR2470
      I=I-1                                                 PTR2480
      IF (I-1-ICX) 399,470,470                                PTR2490
C          NO SOURCE IN ZONE LESS THAN ICY                  PTR2500
C
  500 IF (F2.EQ.0.0) GO TO 510                           PTR2510
      TEMP(1)=H2(I)/RR(NMU)                                 PTR2520
      H4(I)=FREXP(-TEMP(1)-TEMP(1))                         PTR2530
      F2=F2*H4(I)                                         PTR2540
  510 SUMX4(I)=F2                                         PTR2550
      X2(I)=X2(I)-(F2-SUMX3(I))*RR(NGS)                   PTR2560
      I=I-1                                                 PTR2570
      IF (I-IA) 530,500,500                                PTR2580
  520 F2=0.0                                              PTR2590
      GO TO 480                                         PTR2600
  530 CONTINUE                                         PTR2610
      IF (TRDBG .EQ. 0.0 .OR. TRDBG .GE. SOLID(18)) GO TO 539  PTR2620
C          STORE INTENSITIES FOR DEBUG PRINT                PTR2630
      XX = -0.5                                         PTR2640

```

```
      JJJ = JJ + 1          PTR A2750
      WRITE (3)  XX, IAX, JJJ, IBXP1, SOLID(18), TH, RR(NMU)  PTR A2760
      WRITE (3)  (SUMX3(I), SUMX4(I), I = IAX, IBXP1)          PTR A2770
      XX = -2.          PTR A2780
      WRITE (3) (XX, I = 1, 7)          PTR A2790
      BACKSPACE 3          PTR A2800
539  DHNU=HNUP-HNU          PTR A2810
540  JJ = JJ + 1          PTR A2820
      NMU = NMU + 1          PTR A2830
      NGS = NGS + 1          PTR A2840
      IF (JJ-NY) 140,140,550  PTR A2850
550  DO 560 I=IAX,IBXP1          PTR A2860
560  X2(I) = X2(I)* 2.052E12  PTR A2870
      RETURN          PTR A2880
      END          PTR A2890
```

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1. ORIGINATING ACTIVITY (Corporate author) General Atomics Division of General Dynamics Corporation San Diego, California		2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED
		2b. GROUP
3. REPORT TITLE FIREBALL PHENOMENOLOGY AND CODE DEVELOPMENT; Vol IV, SPUTTER Subroutines for Radiation Transport in Planes		
4. DESCRIPTIVE NOTES (Type of report and inclusive dates) 1 June 1963-13 July 1965		
5. AUTHOR(S) (Last name, first name, initial)		
6. REPORT DATE July 1966	7a. TOTAL NO. OF PAGES 62	7b. NO. OF REPS 1
8a. CONTRACT OR GRANT NO. AF 29(601)-6492	8a. ORIGINATOR'S REPORT NUMBER(S) AFWL-TR-65-143, Vol IV	
8b. PROJECT NO. 5710	8b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) GA-6585	
c. Subtask No. 07.003/005		
d.		
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